Evolution of Linear Absorption and Nonlinear Optical Properties in V-Shaped Ruthenium(II)-Based Chromophores

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Supporting Information

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1. Additional Figures

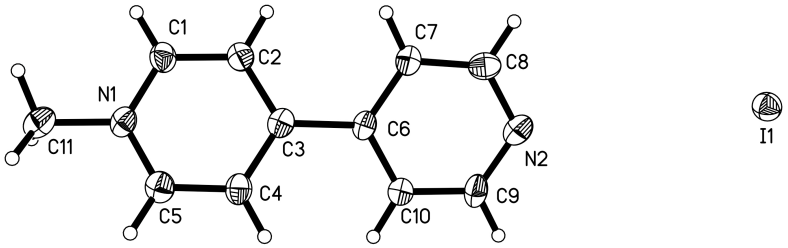


Figure S1. Representation of the molecular structure of the salt [MeQ$^+$]I (50% probability ellipsoids).

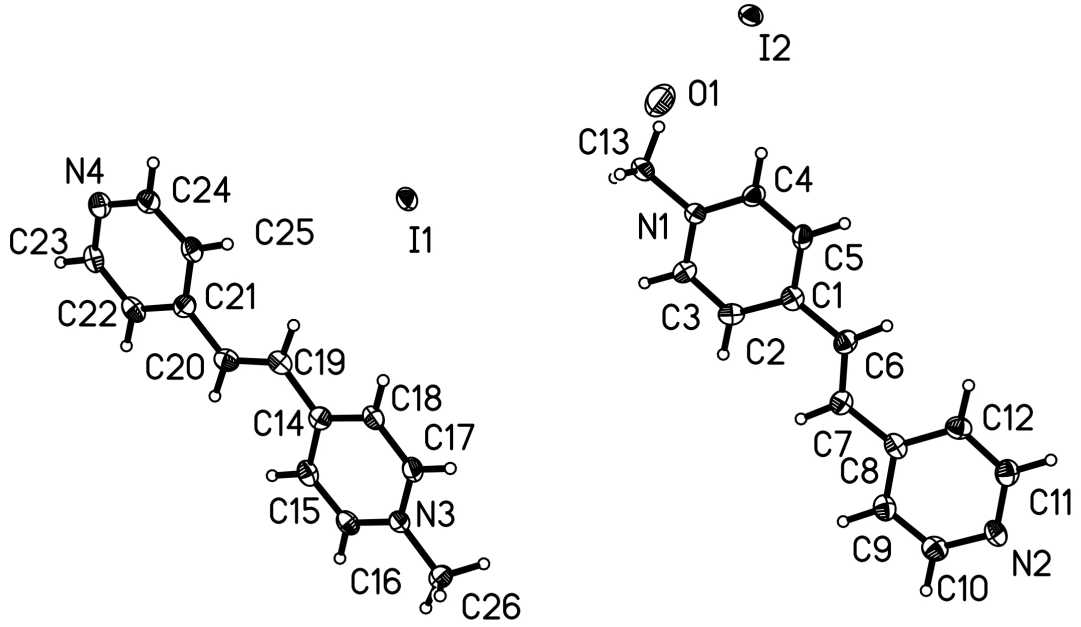


Figure S2. Representation of the molecular structure of the salt [Mebpe$^+$]I•0.5H_2O (50% probability ellipsoids).

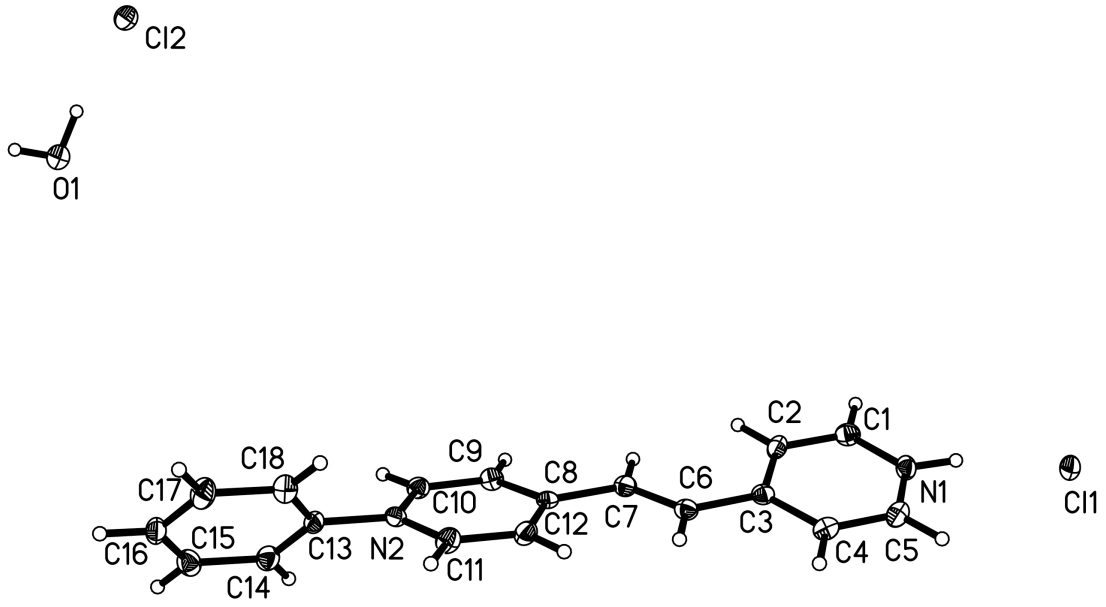


Figure S3. Representation of the molecular structure of the salt [Phbpe^{+}]Cl•HCl•H_2O (50% probability ellipsoids).

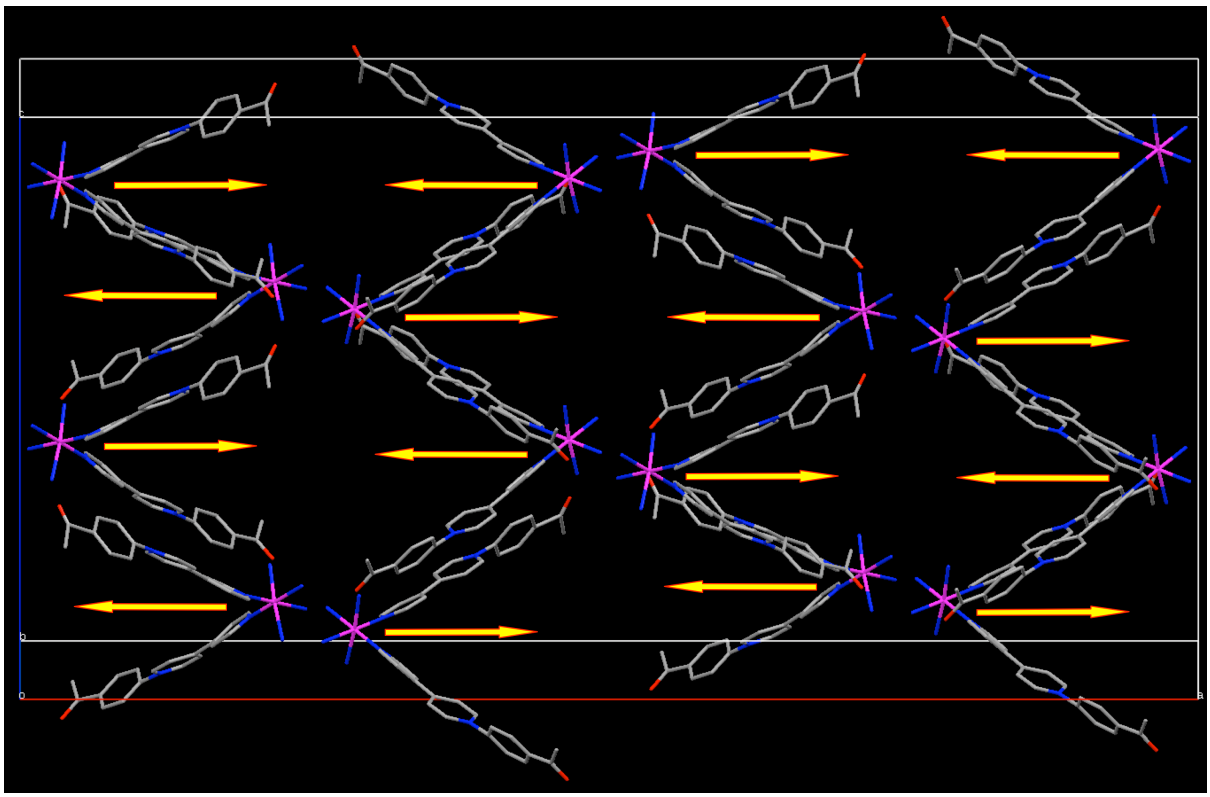


Figure S4. Crystal packing diagram for the salt **3B**, with the BPh_4^- anions and solvents removed for clarity (viewed approximately along the *b* axis). The arrows approximate to the directions of the molecular dipolar axes.

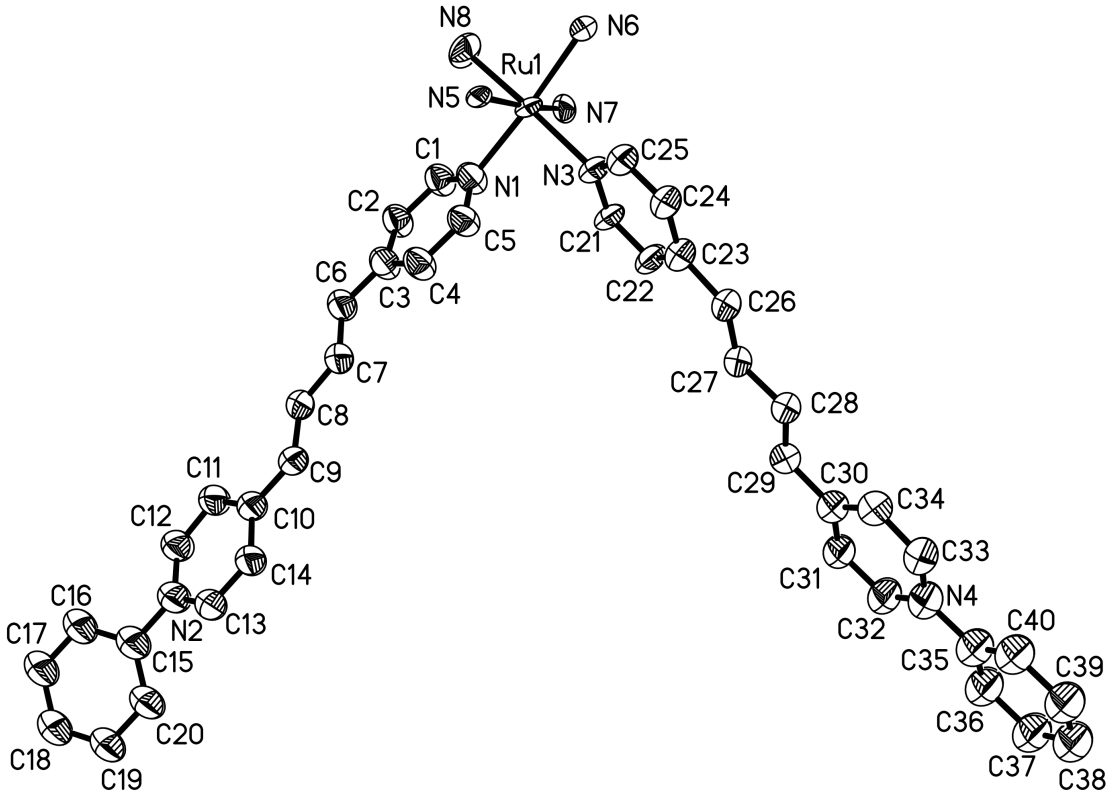


Figure S5. Representation of the molecular structure of the salt **9** (50% probability ellipsoids).

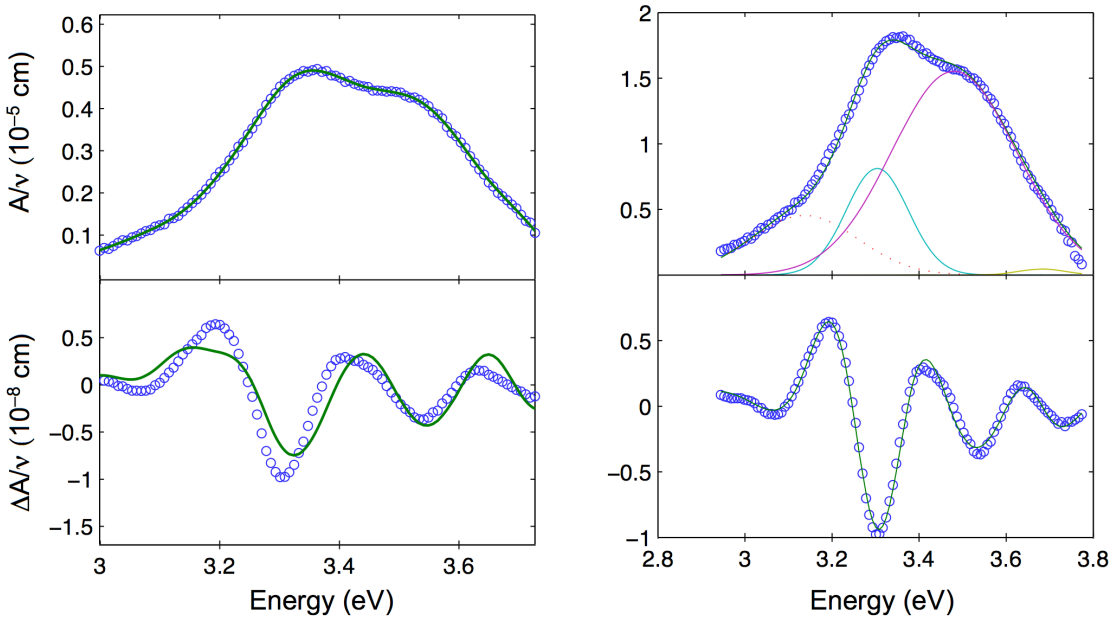


Figure S6. Stark spectra and calculated fits for **8** in an external electric field of 5.36 × 10^7 V m^{-1}, obtained without (left) and with (right) deconvolution. Top panel: absorption spectrum illustrating Gaussian curves used in data fitting; bottom panel: electroabsorption spectrum, experimental (blue) and fits (green) according to the Liptay equation (Liptay, W. In *Excited States*, Vol. 1; Lim, E. C., Ed.; Academic Press, New York, 1974, pp. 129–229).

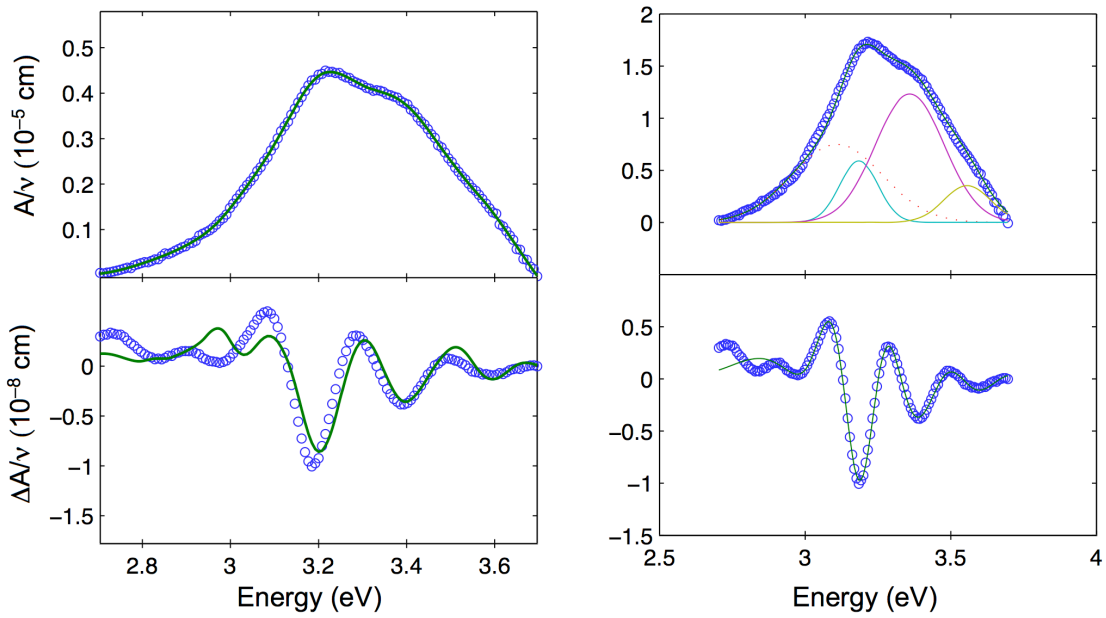


Figure S7. Stark spectra and calculated fits for **9** in an external electric field of 5.36 × 10^7 V m^{-1}, obtained without (left) and with (right) deconvolution. Top panel: absorption spectrum illustrating Gaussian curves used in data fitting; bottom panel: electroabsorption spectrum, experimental (blue) and fits (green) according to the Liptay equation (Liptay, W. In *Excited States*, Vol. 1; Lim, E. C., Ed.; Academic Press, New York, 1974, pp. 129–229).

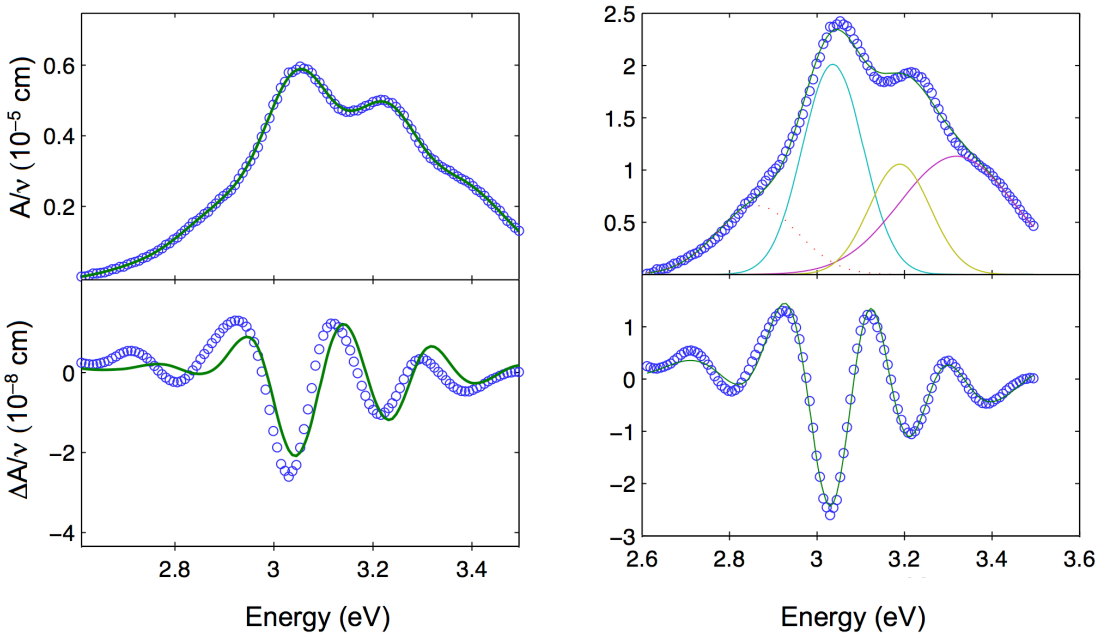


Figure S8. Stark spectra and calculated fits for **10** in an external electric field of 5.36 × 10^7 V m^{-1}, obtained without (left) and with (right) deconvolution. Top panel: absorption spectrum illustrating Gaussian curves used in data fitting; bottom panel: electroabsorption spectrum, experimental (blue) and fits (green) according to the Liptay equation (Liptay, W. In *Excited States*, Vol. 1; Lim, E. C., Ed.; Academic Press, New York, 1974, pp. 129–229).

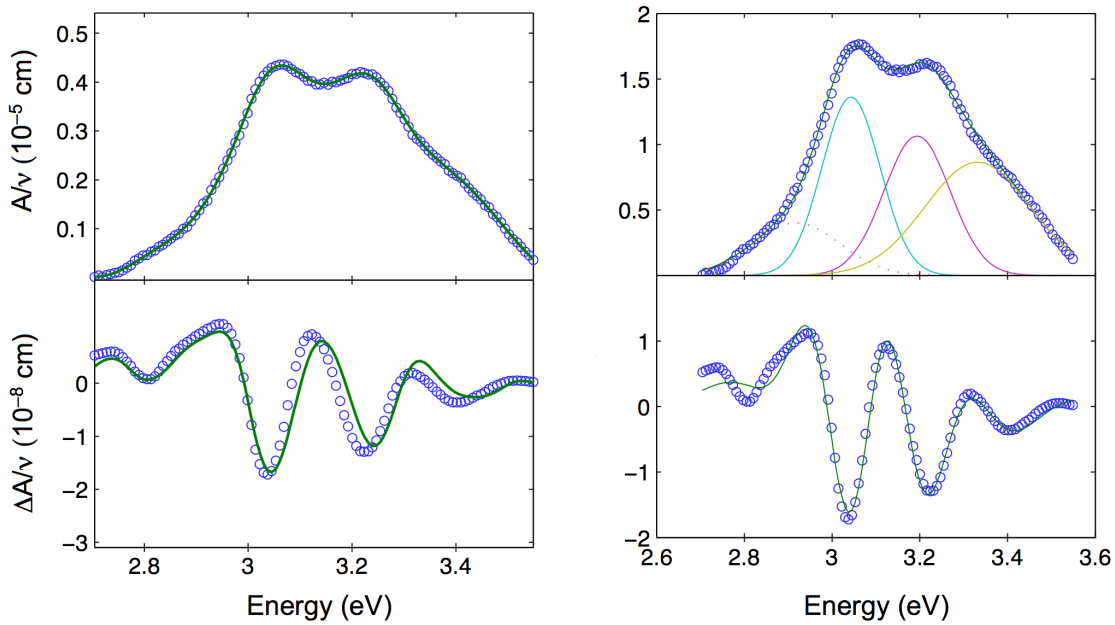


Figure S9. Stark spectra and calculated fits for **11** in an external electric field of 5.36 × 10^7 V m^{-1}, obtained without (left) and with (right) deconvolution. Top panel: absorption spectrum illustrating Gaussian curves used in data fitting; bottom panel: electroabsorption spectrum, experimental (blue) and fits (green) according to the Liptay equation (Liptay, W. In *Excited States*, Vol. 1; Lim, E. C., Ed.; Academic Press, New York, 1974, pp. 129–229).

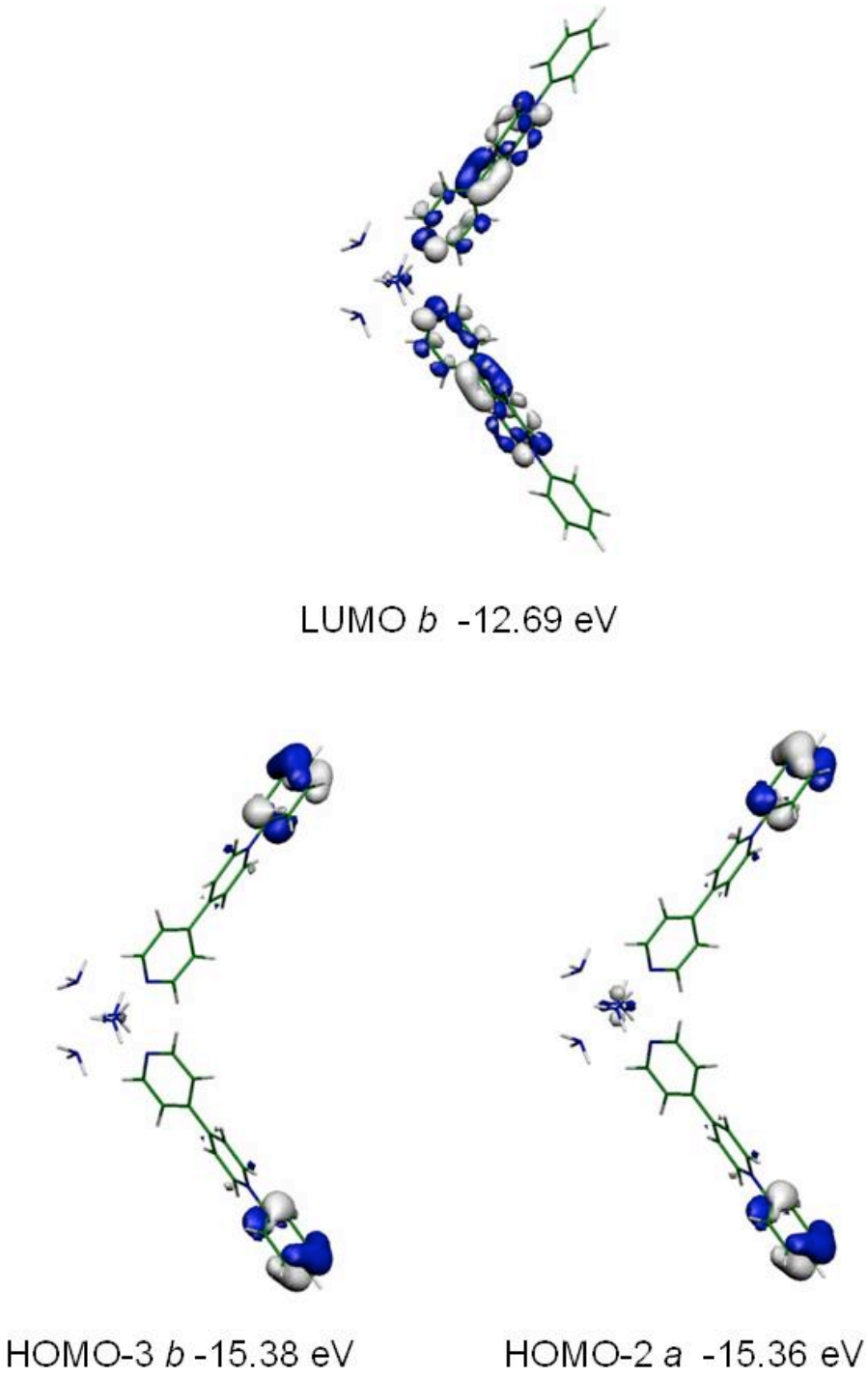
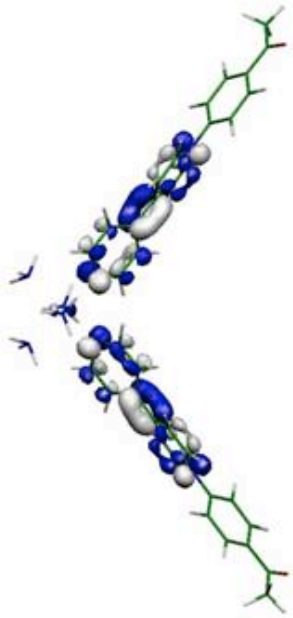
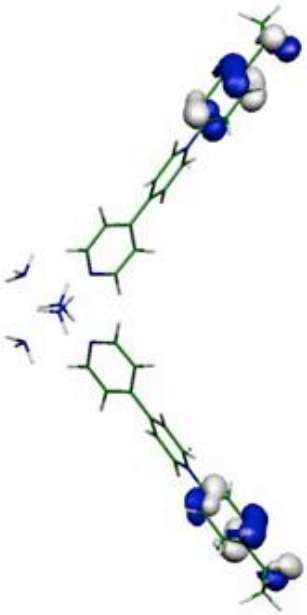


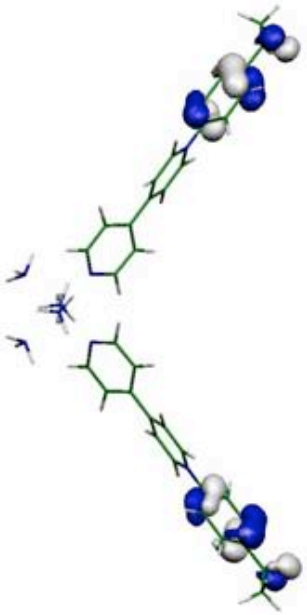
Figure S10. Illustration of the 0.04 contour surface diagrams of the molecular orbitals of **2** involved in the two lowest energy transitions. The axis convention for this and all subsequent Figures is as for Figure 8.



LUMO *b* -12.74 eV



HOMO-3 *b* -15.21 eV



HOMO-2 *a* -15.20 eV

Figure S11. Illustration of the 0.04 contour surface diagrams of the molecular orbitals of **3** involved in the two lowest energy transitions.

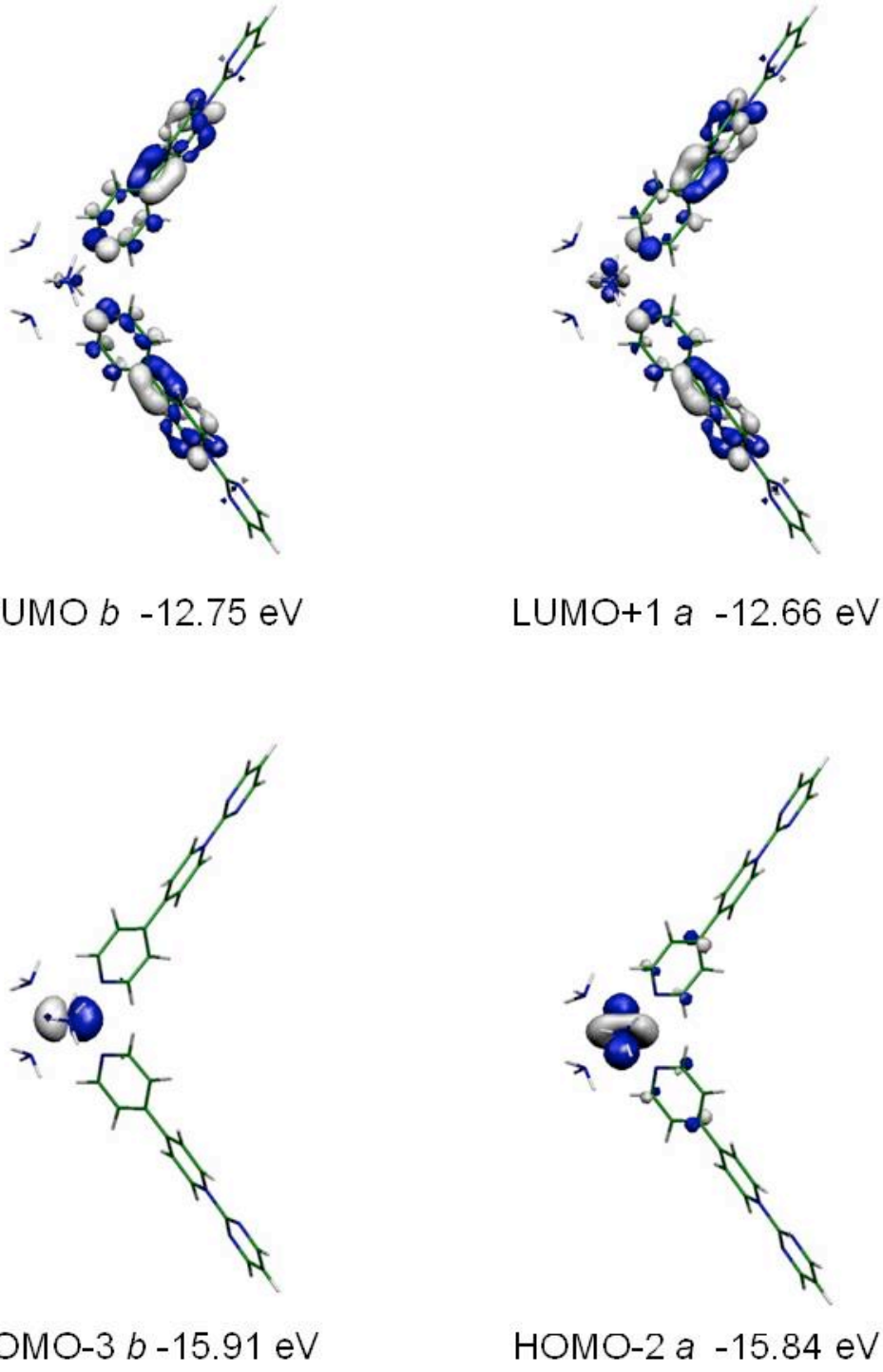


Figure S12. Illustration of the 0.04 contour surface diagrams of the molecular orbitals of **4** involved in the two lowest energy transitions.

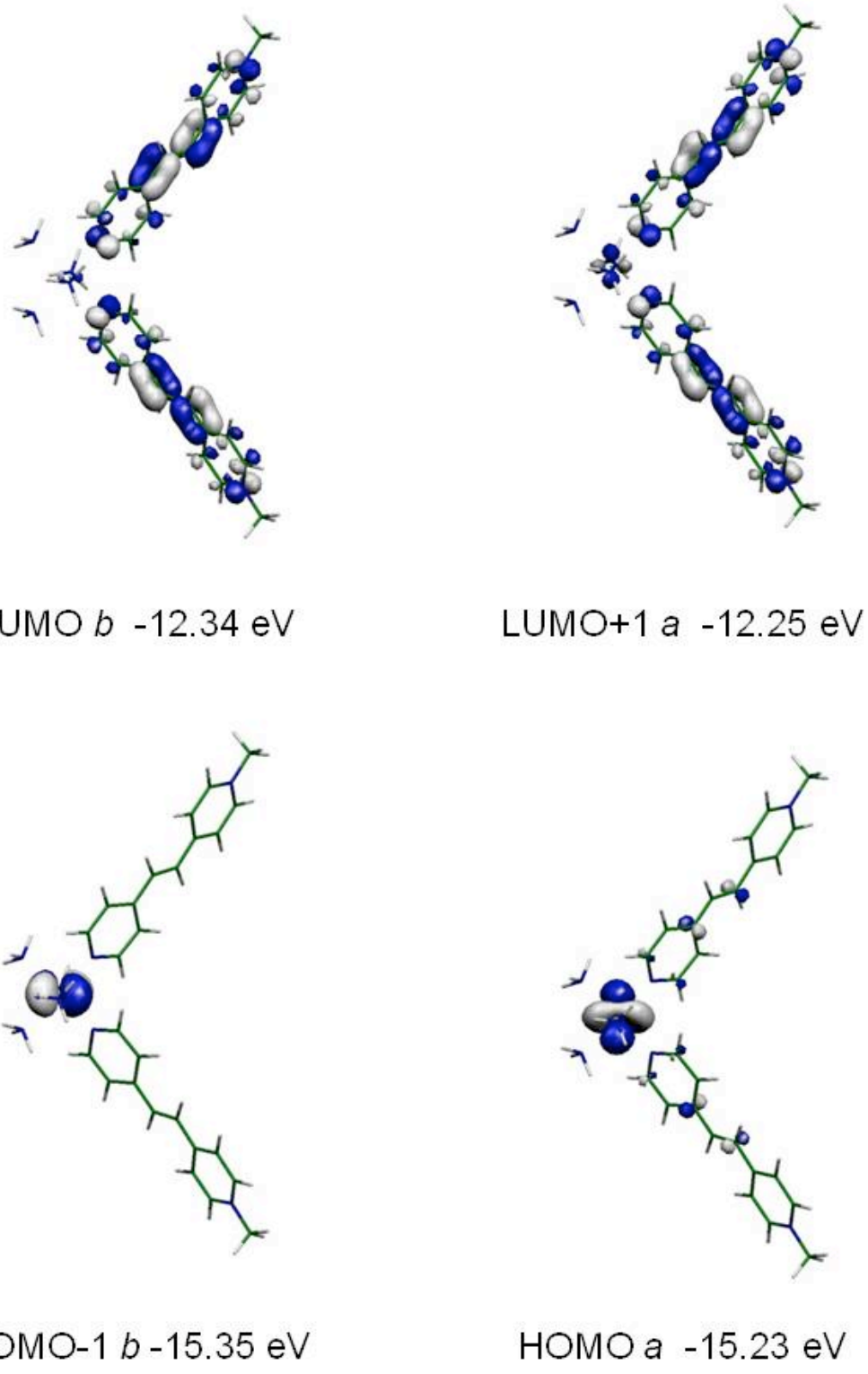


Figure S13. Illustration of the 0.04 contour surface diagrams of the molecular orbitals of **5** involved in the three lowest energy transitions.

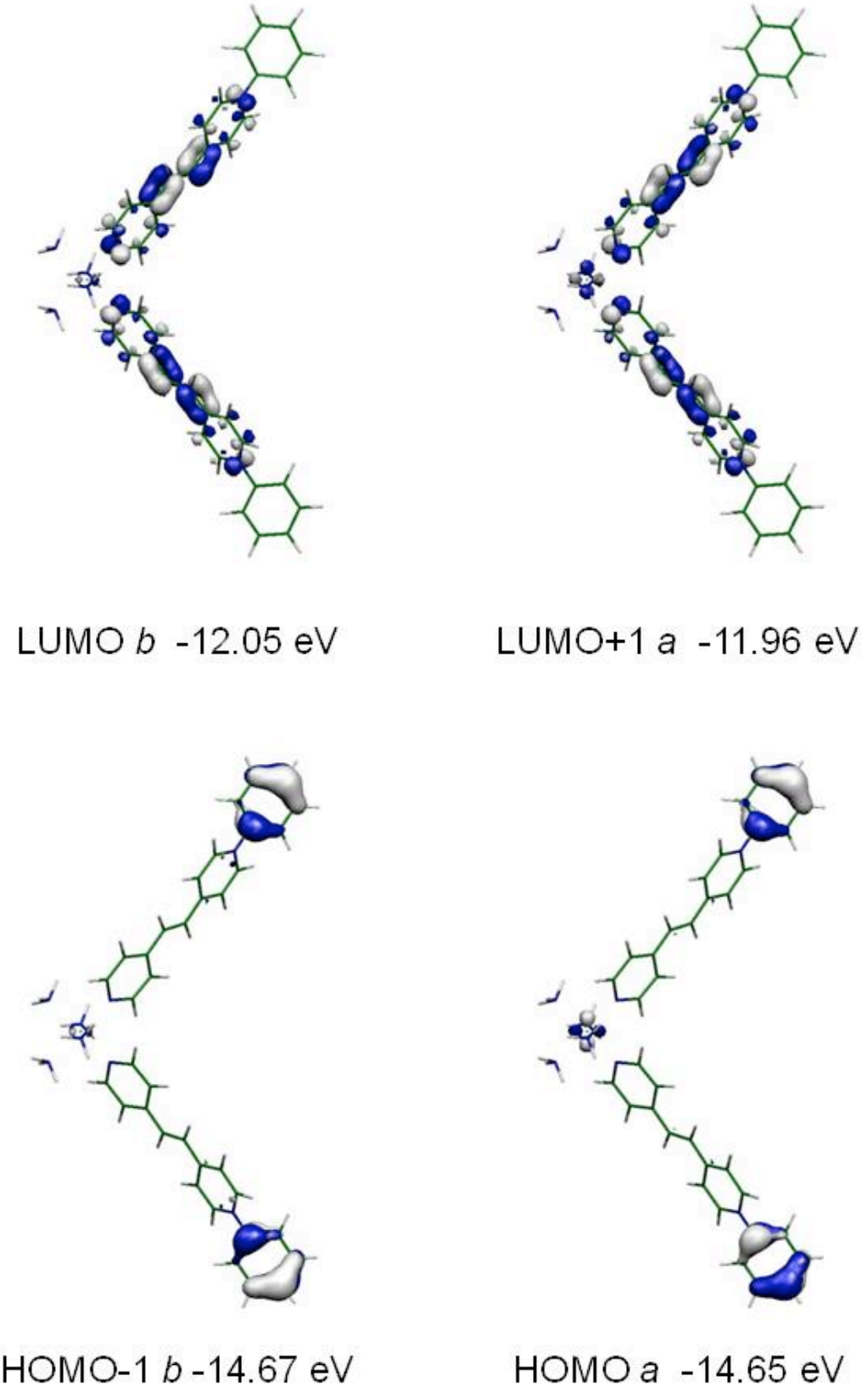


Figure S14. Illustration of the 0.04 contour surface diagrams of the molecular orbitals of **6** involved in the three lowest energy transitions.

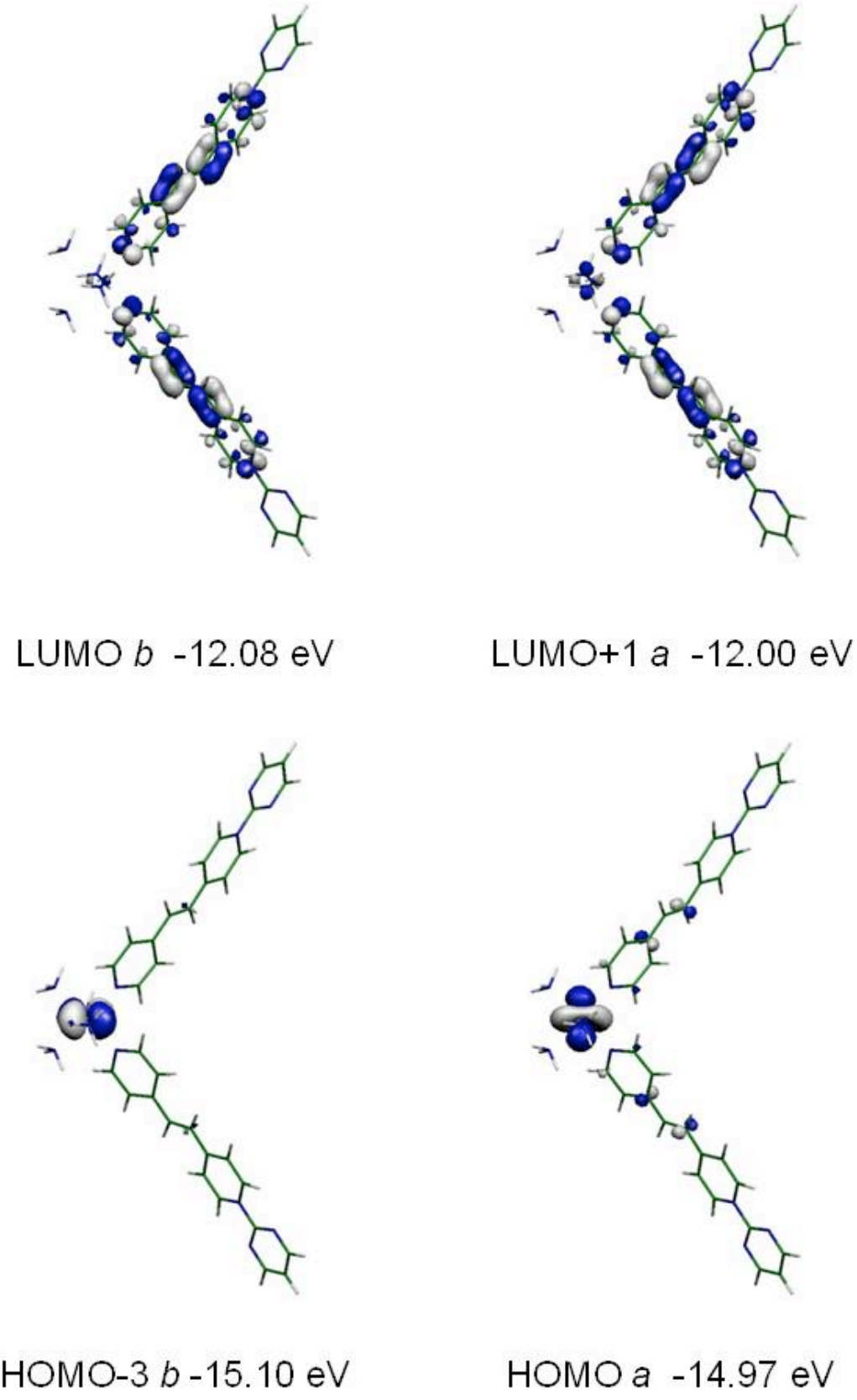


Figure S15. Illustration of the 0.04 contour surface diagrams of the molecular orbitals of **7** involved in the three lowest energy transitions.

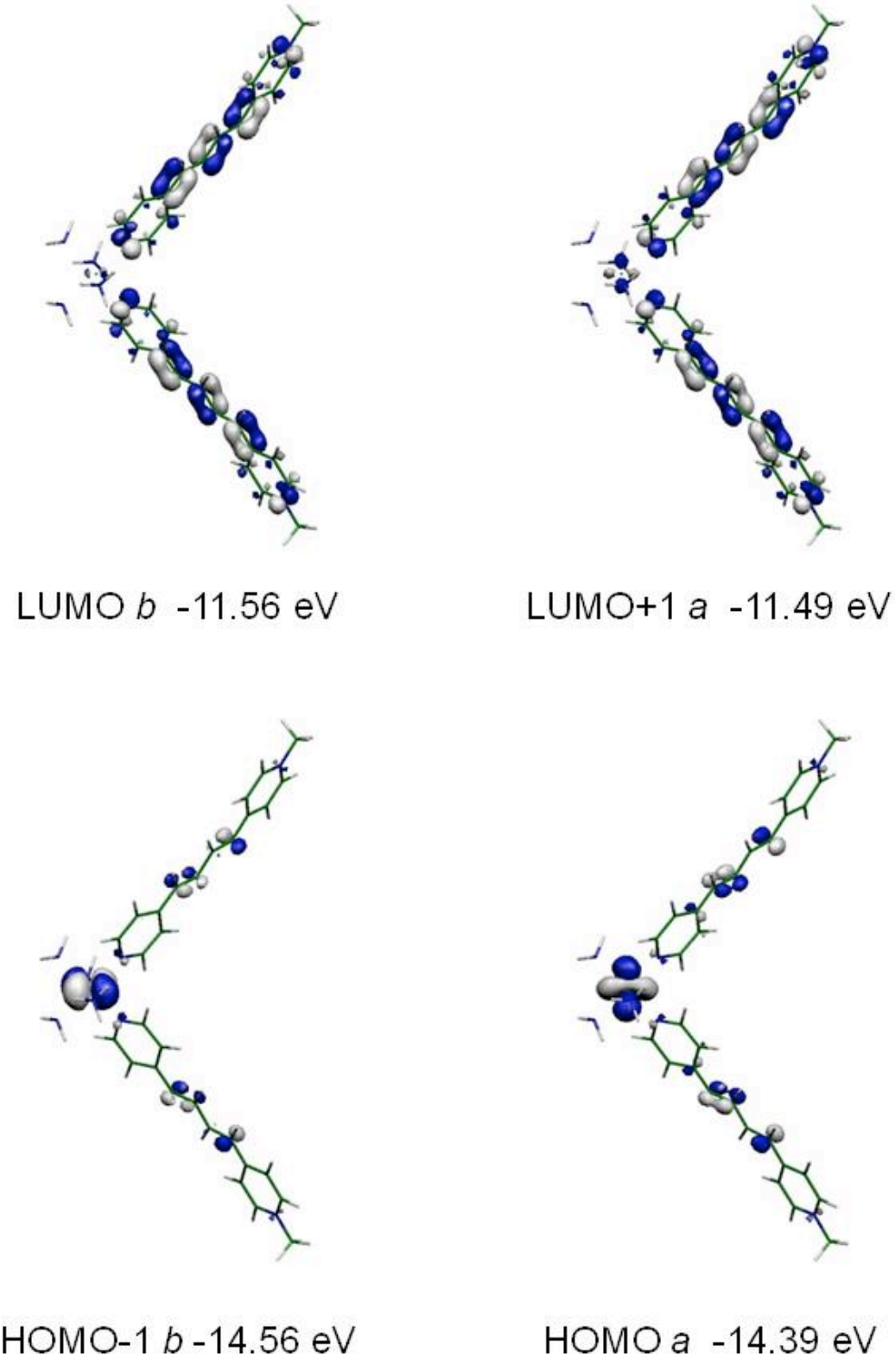


Figure S16. Illustration of the 0.04 contour surface diagrams of the molecular orbitals of **8** involved in the three lowest energy transitions.

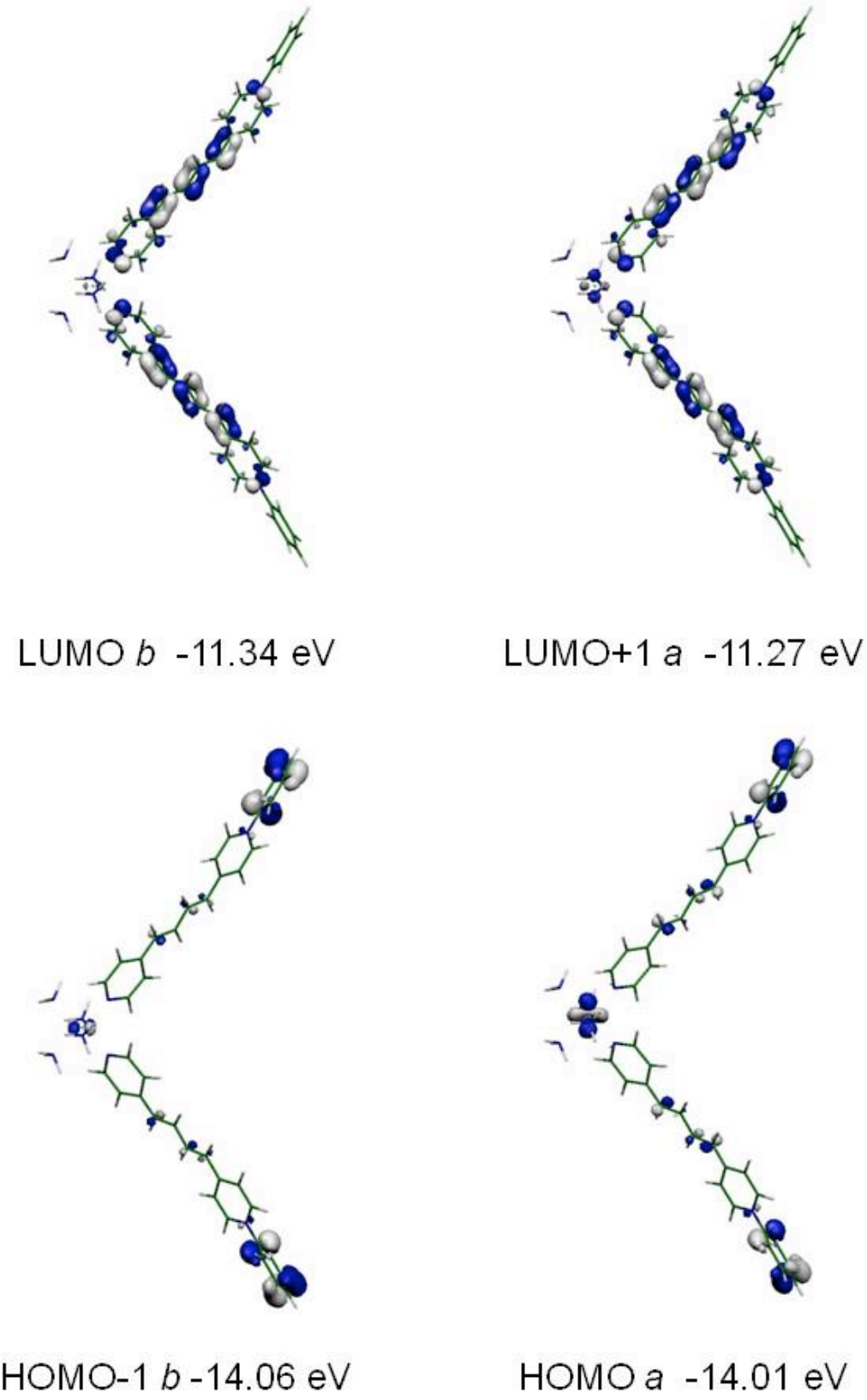


Figure S17. Illustration of the 0.04 contour surface diagrams of the molecular orbitals of **9** involved in the three lowest energy transitions.

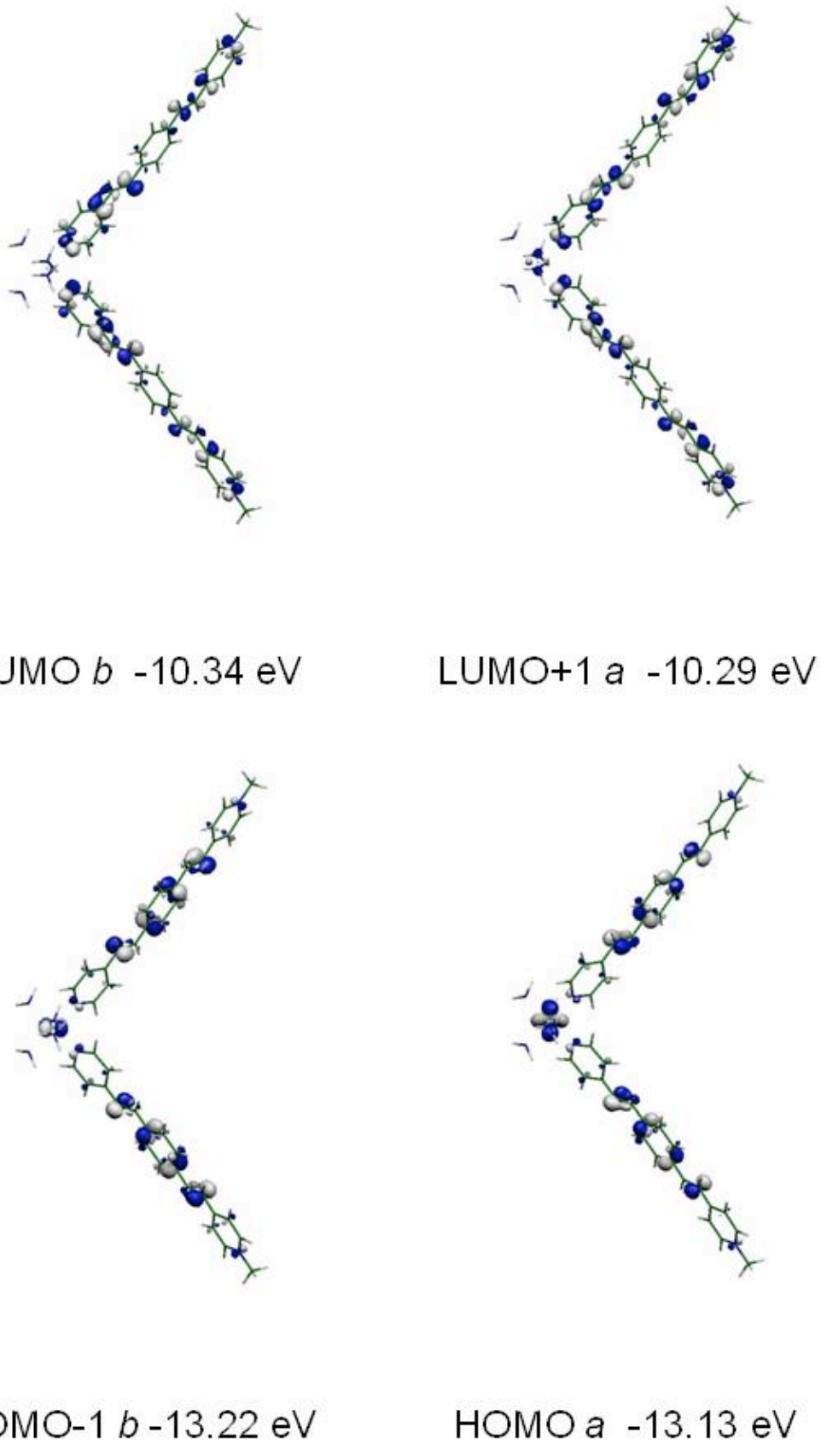


Figure S18. Illustration of the 0.04 contour surface diagrams of the molecular orbitals of **11** involved in the three lowest energy transitions.

2. Additional Tables

Table S1. Selected Interatomic Distances (Å) and Angles (deg) for the Salts [MeQ^+]I, [$Mebpe^+$]I•0.5H_2O and [$Phbpe^+$]Cl•HCl•H_2O

[MeQ^+]I			
C11–N1	1.472(6)	C3–C6	1.480(6)
C1–N1	1.344(6)	C6–C7	1.388(7)
C1–C2	1.366(6)	C7–C8	1.389(6)
C2–C3	1.396(6)	C8–N2	1.342(6)
C3–C4	1.399(7)	C9–N2	1.335(6)
C4–C5	1.364(7)	C9–C10	1.385(6)
C5–N1	1.343(6)	C6–C10	1.391(6)
[$Mebpe^+$]I•0.5H_2O			
C13–N1	1.472(4)	C6–C7	1.328(5)
C3–N1	1.348(5)	C7–C8	1.474(5)
C2–C3	1.365(5)	C8–C9	1.386(5)
C1–C2	1.416(5)	C9–C10	1.376(5)
C1–C5	1.375(5)	C10–N2	1.338(5)
C4–C5	1.369(5)	C11–N2	1.340(5)
C4–N1	1.352(4)	C11–C12	1.388(5)
C1–C6	1.465(5)	C8–C12	1.399(5)
C1–C6–C7	125.7(4)	C6–C7–C8	124.4(4)
C26–N3	1.469(5)	C19–C20	1.334(5)
C16–N3	1.358(4)	C20–C21	1.464(5)
C15–C16	1.367(5)	C21–C22	1.398(5)
C14–C15	1.404(5)	C22–C23	1.380(5)
C14–C18	1.393(5)	C23–N4	1.339(5)
C17–C18	1.356(5)	C24–N4	1.339(5)
C17–N3	1.346(5)	C24–C25	1.380(5)
C14–C19	1.461(5)	C21–C25	1.397(5)
C14–C19–C20	124.3(4)	C19–C20–C21	125.1(4)
[$Phbpe^+$]Cl•HCl•H_2O			
C1–N1	1.352(4)	C7–C8	1.467(4)
C1–C2	1.378(4)	C8–C9	1.400(4)
C2–C3	1.401(4)	C9–C10	1.372(4)
C3–C4	1.397(4)	C10–N2	1.344(4)
C4–C5	1.365(4)	C11–N2	1.352(4)
C5–N1	1.340(4)	C11–C12	1.370(4)
C3–C6	1.462(4)	C8–C12	1.398(4)
C6–C7	1.333(4)	C13–N2	1.454(3)
C3–C6–C7	124.3(3)	C6–C7–C8	124.7(3)

Table S2. Crystallographic Data and Refinement Details for the Salt **9**

	9•MeCN•H_2O
formula	$C_{40}H_{46}F_{24}N_8P_4Ru$
M	1319.80
crystal system	monoclinic
space group	*Cc*
a/Å	25.521(17)
b/Å	14.223(10)
c/Å	15.130(10)
β/°	113.409(13)
U/Å^3	5040(6)
Z	4
T/K	100(2)
μ/mm^{-1}	0.568
crystal size/mm^3	0.30 × 0.10 × 0.10
crystal appearance	black prism
reflections collected	7928
independent reflections (R_{int})	3424 (0.1541)
reflections with $I > 2\sigma(I)$	1789
goodness-of-fit on F^2	1.040
final $R1$, $wR2$ [$I > 2\sigma(I)$][a]	0.1104, 0.2623
(all data)	0.1911, 0.3121
peak and hole (e Å^{-3})	0.798, –0.496

[a] The structure was refined on F_o^2 using all data; the values of $R1$ are given for comparison with older refinements based on F_o with a typical threshold of $F_o > 4\sigma(F_o)$.

Table S3. ILCT Absorption and Stark Spectroscopic Data for Complex Salts **8**–**11**[a]

salt (L^A)	λ_{max}[b] (nm)	E_{max}[b] (eV)	f_{os}[b]	μ_{12}[c] (D)	$\Delta\mu_{12}$[d] (D)	$\Delta\mu_{ab}$[e] (D)	r_{12}[f] (Å)	r_{ab}[g] (Å)	c_b^2[h]	H_{ab}[i] (10^3 cm^{-1})	β_0[j] (10^{-30} esu)	$\Sigma[\beta_0]_{ICT}$[k] (10^{-30} esu)
8 (Mebpb$^+$)	395	3.14	0.15	3.6	12.3	14.3	2.6	3.0	0.93	6.4	18	84
	375	3.3	0.17	3.7	11.8	13.9	2.4	2.9	0.92	7.0	16	
	356	3.48	0.67	7.2	9.9	17.5	2.1	3.6	0.78	11.5	50	
	337	3.68	0.01	0.8	6.1	6.3	1.3	1.3	0.99	3.5	<1	
	369	3.36	0.95	8.7	11.3	20.7	2.3	4.3	0.77	11.4	88	
9 (Phbpb$^+$)	399	3.11	0.35	5.5	15.1	18.6	3.1	3.9	0.91	7.3	54	120
	389	3.18	0.12	3.1	12.2	13.7	2.5	2.9	0.94	5.9	14	
	369	3.36	0.47	6.1	12.0	17.1	2.5	3.6	0.85	9.7	46	
	349	3.56	0.10	2.7	8.7	10.2	1.8	2.1	0.93	7.5	6	
	385	3.22	1.02	9.2	11.9	21.9	2.5	4.5	0.77	10.9	112	
10 (Mebph$^+$)	433	2.86	0.16	3.9	12.3	14.5	2.6	3.0	0.92	6.1	26	164
	408	3.04	0.39	5.9	12.4	17.1	2.6	3.6	0.86	8.4	54	
	389	3.19	0.22	4.3	13.5	16.0	2.8	3.3	0.92	6.9	28	
	374	3.32	0.45	6.0	14.5	18.9	3.0	3.9	0.89	8.5	56	
	407	3.05	1.33	10.7	11.0	24.1	2.3	5.0	0.73	11.0	158	
11 (Mebpvb$^+$)	425	2.92	0.16	3.8	14.5	16.4	3.0	3.4	0.94	5.5	28	183
	407	3.04	0.38	5.7	12.8	17.2	2.7	3.6	0.87	8.1	53	
	388	3.19	0.35	5.4	14.5	18.1	3.0	3.8	0.90	7.7	48	
	372	3.33	0.47	6.1	13.8	18.5	2.9	3.8	0.87	9.0	54	
	405	3.06	1.34	10.8	12.7	25.0	2.6	5.2	0.76	10.6	184	

[a] Measured in butyronitrile glasses at 77 K. [b] For the four fitted Gaussian components of the ILCT bands; f_{os} values were obtained from $(4.60 \times 10^{-9}$ M $cm^2)\varepsilon_{max} \times fw_{1/2}$ where ε_{max} is the maximal molar extinction coefficient and $fw_{1/2}$ is the full width at half height (in wavenumbers). The experimentally observed data are highlighted in yellow; f_{os} values were obtained from $(4.32 \times 10^{-9}$ M $cm^2)A$ where A is the numerically integrated area under the absorption peak. [c] Calculated from eq 2. [d] Calculated from $f_{int}\Delta\mu_{12}$ using $f_{int} = 1.33$. [e] Calculated from eq 1. [f] Delocalized electron-transfer distance calculated from $\Delta\mu_{12}/e$. [g] Effective (localized) electron-transfer distance calculated from $\Delta\mu_{ab}/e$. [h] Calculated from eq 3. [i] Calculated from eq 4. [j] Calculated from eq 5. [k] The sum of the individual β_0 components for the ILCT bands; the values in red in the preceding column are the comparable (and very similar) NLO responses determined without spectral deconvolution.

3. Cartesian Coordinates of Theoretically Optimized Geometries

Complex cation 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.067940	1.541531	1.125966
2	6	0	-0.749260	1.572956	0.027973
3	6	0	0.877334	2.632051	1.307848
4	6	0	0.872612	3.744402	0.465991
5	6	0	0.000000	3.793748	-0.641661
6	6	0	-0.812727	2.658376	-0.849217
7	7	0	-0.067940	-1.541531	1.125966
8	44	0	0.000000	0.000000	2.550230
9	6	0	-0.877334	-2.632051	1.307848
10	6	0	-0.872612	-3.744402	0.465991
11	6	0	0.000000	-3.793748	-0.641661
12	6	0	0.812727	-2.658376	-0.849217
13	6	0	0.749260	-1.572956	0.027973
14	6	0	0.063693	-4.984982	-1.527635
15	6	0	1.270964	-5.377839	-2.144663
16	6	0	1.312434	-6.509218	-2.954537
17	7	0	0.194232	-7.256314	-3.170361
18	6	0	-0.988242	-6.902224	-2.593348
19	6	0	-1.076365	-5.780584	-1.774940
20	6	0	0.268344	-8.489201	-4.014304
21	6	0	-0.063693	4.984982	-1.527635
22	6	0	-1.270964	5.377839	-2.144663
23	6	0	-1.312434	6.509218	-2.954537
24	7	0	-0.194232	7.256314	-3.170361
25	6	0	0.988242	6.902224	-2.593348
26	6	0	1.076365	5.780584	-1.774940
27	6	0	-0.268344	8.489201	-4.014304
28	7	0	2.163510	-0.153366	2.553641
29	7	0	-0.041916	-1.515230	4.128543
30	7	0	0.041916	1.515230	4.128543
31	7	0	-2.163510	0.153366	2.553641
32	1	0	1.359860	-0.695227	-0.146128
33	1	0	-1.359860	0.695227	-0.146128
34	1	0	1.525494	4.575598	0.710334
35	1	0	-1.483344	2.593139	-1.699542
36	1	0	-1.536585	-2.615075	2.167720
37	1	0	-1.525494	-4.575598	0.710334
38	1	0	1.483344	-2.593139	-1.699542
39	1	0	2.196483	-4.837124	-1.986500
40	1	0	2.226316	-6.842556	-3.430629
41	1	0	-1.845444	-7.529896	-2.804187
42	1	0	-2.047432	-5.533259	-1.362798
43	1	0	0.444395	-9.355982	-3.372278
44	1	0	-0.669011	-8.614005	-4.557714
45	1	0	1.083046	-8.390081	-4.732002
46	1	0	-2.196483	4.837124	-1.986500
47	1	0	-2.226316	6.842556	-3.430629
48	1	0	1.845444	7.529896	-2.804187
49	1	0	2.047432	5.533259	-1.362798

50	1	0	-1.083046	8.390081	-4.732002
51	1	0	-0.444395	9.355982	-3.372278
52	1	0	0.669011	8.614005	-4.557714
53	1	0	2.591351	0.003422	3.471956
54	1	0	2.446407	-1.090294	2.249253
55	1	0	0.574392	-1.261891	4.907524
56	1	0	-0.971926	-1.670175	4.530823
57	1	0	0.971926	1.670175	4.530823
58	1	0	-0.285799	2.418579	3.771887
59	1	0	-2.446407	1.090294	2.249253
60	1	0	-2.586005	-0.516943	1.903665
61	1	0	-2.591351	-0.003422	3.471956
62	1	0	-0.574392	1.261891	4.907524
63	1	0	2.586005	0.516943	1.903665
64	1	0	0.285799	-2.418579	3.771887
65	1	0	1.536585	2.615075	2.167720

Complex cation 2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.120051	1.532307	2.119368
2	6	0	-0.694828	1.581152	1.019933
3	6	0	0.959119	2.601120	2.295724
4	6	0	0.984401	3.708944	1.449209
5	6	0	0.113867	3.778988	0.340065
6	6	0	-0.727598	2.662866	0.137853
7	7	0	-0.120051	-1.532307	2.119368
8	44	0	0.000000	0.000000	3.546524
9	6	0	-0.959119	-2.601120	2.295724
10	6	0	-0.984401	-3.708944	1.449209
11	6	0	-0.113867	-3.778988	0.340065
12	6	0	0.727598	-2.662866	0.137853
13	6	0	0.694828	-1.581152	1.019933
14	6	0	-0.079910	-4.966100	-0.548393
15	6	0	1.109496	-5.369101	-1.194418
16	6	0	1.126465	-6.493327	-2.010538
17	7	0	0.000000	-7.247083	-2.195990
18	6	0	-1.166903	-6.883785	-1.581154
19	6	0	-1.228944	-5.756166	-0.772053
20	6	0	0.079910	4.966100	-0.548393
21	6	0	-1.109496	5.369101	-1.194418
22	6	0	-1.126465	6.493327	-2.010538
23	7	0	0.000000	7.247083	-2.195990
24	6	0	1.166903	6.883785	-1.581154
25	6	0	1.228944	5.756166	-0.772053
26	7	0	2.155473	-0.236003	3.544329
27	7	0	-0.096960	-1.516973	5.121690
28	7	0	0.096960	1.516973	5.121690
29	7	0	-2.155473	0.236003	3.544329
30	1	0	-1.327830	0.718774	0.848554
31	1	0	1.659142	4.523179	1.690547
32	1	0	-1.398401	2.610902	-0.713057
33	1	0	-1.617643	-2.571026	3.155994
34	1	0	-1.659142	-4.523179	1.690547
35	1	0	1.398401	-2.610902	-0.713057
36	1	0	2.039943	-4.828764	-1.065812
37	1	0	2.011838	-6.807976	-2.547283

38	1	0	-2.017918	-7.533804	-1.736946
39	1	0	-2.186729	-5.510168	-0.328886
40	1	0	-2.039943	4.828764	-1.065812
41	1	0	-2.011838	6.807976	-2.547283
42	1	0	2.017918	7.533804	-1.736946
43	1	0	2.186729	5.510168	-0.328886
44	1	0	2.589272	-0.138034	4.467711
45	1	0	2.396900	-1.169646	3.197223
46	1	0	0.521201	-1.284393	5.905353
47	1	0	-1.034272	-1.645947	5.515700
48	1	0	1.034272	1.645947	5.515700
49	1	0	-0.206780	2.427025	4.761063
50	1	0	-2.396900	1.169646	3.197223
51	1	0	-2.604448	-0.444460	2.923290
52	1	0	-2.589272	0.138034	4.467711
53	1	0	-0.521201	1.284393	5.905353
54	1	0	2.604448	0.444460	2.923290
55	1	0	0.206780	-2.427025	4.761063
56	1	0	1.617643	2.571026	3.155994
57	1	0	1.327830	-0.718774	0.848554
58	6	0	0.043796	-8.432375	-3.041348
59	6	0	-0.997294	-8.655258	-3.959711
60	6	0	1.125048	-9.322336	-2.913928
61	6	0	-0.947398	-9.797347	-4.766846
62	1	0	-1.804470	-7.939039	-4.086791
63	6	0	1.157526	-10.459765	-3.728516
64	1	0	1.899456	-9.170771	-2.166961
65	6	0	0.125735	-10.698814	-4.653335
66	1	0	-1.733261	-9.976997	-5.492002
67	1	0	1.974325	-11.166265	-3.631316
68	1	0	0.157380	-11.582737	-5.280941
69	6	0	-0.043796	8.432375	-3.041348
70	6	0	0.997294	8.655258	-3.959711
71	6	0	-1.125048	9.322336	-2.913928
72	6	0	0.947398	9.797347	-4.766846
73	1	0	1.804470	7.939039	-4.086791
74	6	0	-1.157526	10.459765	-3.728516
75	1	0	-1.899456	9.170771	-2.166961
76	6	0	-0.125735	10.698814	-4.653335
77	1	0	1.733261	9.976997	-5.492002
78	1	0	-1.974325	11.166265	-3.631316
79	1	0	-0.157380	11.582737	-5.280941

Complex cation 3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.125081	1.531711	2.837755
2	6	0	-0.693237	1.584203	1.741000
3	6	0	0.970382	2.596179	3.010828
4	6	0	0.999596	3.702939	2.162861
5	6	0	0.125697	3.776593	1.056672
6	6	0	-0.723364	2.665612	0.858396
7	7	0	-0.125081	-1.531711	2.837755
8	44	0	0.000000	0.000000	4.265370
9	6	0	-0.970382	-2.596179	3.010828
10	6	0	-0.999596	-3.702939	2.162861

11	6	0	-0.125697	-3.776593	1.056672
12	6	0	0.723364	-2.665612	0.858396
13	6	0	0.693237	-1.584203	1.741000
14	6	0	-0.097554	-4.961322	0.164742
15	6	0	1.093928	-5.378852	-0.468623
16	6	0	1.103245	-6.496888	-1.293244
17	7	0	-0.033700	-7.228948	-1.500377
18	6	0	-1.202376	-6.853005	-0.896094
19	6	0	-1.255876	-5.732152	-0.077118
20	6	0	0.097554	4.961322	0.164742
21	6	0	-1.093928	5.378852	-0.468623
22	6	0	-1.103245	6.496888	-1.293244
23	7	0	0.033700	7.228948	-1.500377
24	6	0	1.202376	6.853005	-0.896094
25	6	0	1.255876	5.732152	-0.077118
26	7	0	2.154584	-0.244667	4.264428
27	7	0	-0.103656	-1.516681	5.840106
28	7	0	0.103656	1.516681	5.840106
29	7	0	-2.154584	0.244667	4.264428
30	1	0	-1.331025	0.724902	1.571959
31	1	0	1.680017	4.513551	2.400632
32	1	0	-1.397221	2.617122	0.009657
33	1	0	-1.631079	-2.563508	3.869340
34	1	0	-1.680017	-4.513551	2.400632
35	1	0	1.397221	-2.617122	0.009657
36	1	0	2.030820	-4.853904	-0.323892
37	1	0	1.990120	-6.821877	-1.821365
38	1	0	-2.062348	-7.486472	-1.070354
39	1	0	-2.214768	-5.474062	0.356743
40	1	0	-2.030820	4.853904	-0.323892
41	1	0	-1.990120	6.821877	-1.821365
42	1	0	2.062348	7.486472	-1.070354
43	1	0	2.214768	5.474062	0.356743
44	1	0	2.587213	-0.152333	5.188956
45	1	0	2.392653	-1.178007	3.914154
46	1	0	0.518323	-1.289230	6.622265
47	1	0	-1.040829	-1.638707	6.236690
48	1	0	1.040829	1.638707	6.236690
49	1	0	-0.192153	2.428894	5.478326
50	1	0	-2.392653	1.178007	3.914154
51	1	0	-2.607989	-0.436090	3.646977
52	1	0	-2.587213	0.152333	5.188956
53	1	0	-0.518323	1.289230	6.622265
54	1	0	2.607989	0.436090	3.646977
55	1	0	0.192153	-2.428894	5.478326
56	1	0	1.631079	2.563508	3.869340
57	1	0	1.331025	-0.724902	1.571959
58	6	0	-0.005127	-8.399253	-2.366174
59	6	0	-1.036676	-8.575925	-3.306733
60	6	0	1.046423	-9.321975	-2.240861
61	6	0	-1.003511	-9.698119	-4.132756
62	1	0	-1.821845	-7.835031	-3.430949
63	6	0	1.061073	-10.444184	-3.077453
64	1	0	1.813012	-9.206620	-1.479526
65	6	0	0.041474	-10.640976	-4.027947
66	1	0	-1.768583	-9.868810	-4.884310
67	1	0	1.860629	-11.169591	-2.972880
68	6	0	0.005127	8.399253	-2.366174
69	6	0	1.036676	8.575925	-3.306733
70	6	0	-1.046423	9.321975	-2.240861
71	6	0	1.003511	9.698119	-4.132756

72	1	0	1.821845	7.835031	-3.430949
73	6	0	-1.061073	10.444184	-3.077453
74	1	0	-1.813012	9.206620	-1.479526
75	6	0	-0.041474	10.640976	-4.027947
76	1	0	1.768583	9.868810	-4.884310
77	1	0	-1.860629	11.169591	-2.972880
78	6	0	0.000000	11.834583	-4.963732
79	8	0	0.950003	11.906161	-5.764949
80	6	0	0.000000	-11.834583	-4.963732
81	8	0	-0.950003	-11.906161	-5.764949
82	6	0	1.084845	-12.872808	-4.892736
83	1	0	2.071893	-12.432829	-5.081158
84	1	0	1.112707	-13.350480	-3.905373
85	1	0	0.896198	-13.640356	-5.643974
86	6	0	-1.084845	12.872808	-4.892736
87	1	0	-2.071893	12.432829	-5.081158
88	1	0	-1.112707	13.350480	-3.905373
89	1	0	-0.896198	13.640356	-5.643974

Complex cation 4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.092705	1.533644	2.100886
2	6	0	-0.724417	1.568879	1.002861
3	6	0	0.916671	2.614094	2.276185
4	6	0	0.925660	3.721223	1.428083
5	6	0	0.052365	3.776205	0.320930
6	6	0	-0.774333	2.649596	0.119980
7	7	0	-0.092705	-1.533644	2.100886
8	44	0	0.000000	0.000000	3.528101
9	6	0	-0.916671	-2.614094	2.276185
10	6	0	-0.925660	-3.721223	1.428083
11	6	0	-0.052365	-3.776205	0.320930
12	6	0	0.774333	-2.649596	0.119980
13	6	0	0.724417	-1.568879	1.002861
14	6	0	0.000000	-4.963252	-0.568600
15	6	0	1.206784	-5.362350	-1.185361
16	6	0	1.246411	-6.492443	-1.991786
17	7	0	0.114507	-7.226105	-2.198651
18	6	0	-1.073808	-6.871022	-1.629105
19	6	0	-1.148351	-5.748489	-0.814787
20	6	0	0.000000	4.963252	-0.568600
21	6	0	-1.206784	5.362350	-1.185361
22	6	0	-1.246411	6.492443	-1.991786
23	7	0	-0.114507	7.226105	-2.198651
24	6	0	1.073808	6.871022	-1.629105
25	6	0	1.148351	5.748489	-0.814787
26	7	0	2.159676	-0.194718	3.526636
27	7	0	-0.069562	-1.518430	5.103373
28	7	0	0.069562	1.518430	5.103373
29	7	0	-2.159676	0.194718	3.526636
30	1	0	-1.345221	0.697328	0.833678
31	1	0	1.589175	4.545846	1.665514
32	1	0	-1.446081	2.589681	-0.729723
33	1	0	-1.575902	-2.593425	3.136150
34	1	0	-1.589175	-4.545846	1.665514

35	1	0	1.446081	-2.589681	-0.729723
36	1	0	2.134391	-4.826413	-1.023388
37	1	0	2.136002	-6.866627	-2.485678
38	1	0	-1.910958	-7.518366	-1.864706
39	1	0	-2.116008	-5.490294	-0.401348
40	1	0	-2.134391	4.826413	-1.023388
41	1	0	-2.136002	6.866627	-2.485678
42	1	0	1.910958	7.518366	-1.864706
43	1	0	2.116008	5.490294	-0.401348
44	1	0	2.592147	-0.073094	4.447883
45	1	0	2.420642	-1.128486	3.194246
46	1	0	0.547737	-1.277022	5.885087
47	1	0	-1.003545	-1.661128	5.500569
48	1	0	1.003545	1.661128	5.500569
49	1	0	-0.246098	2.424116	4.741937
50	1	0	-2.420642	1.128486	3.194246
51	1	0	-2.593953	-0.484986	2.894406
52	1	0	-2.592147	0.073094	4.447883
53	1	0	-0.547737	1.277022	5.885087
54	1	0	2.593953	0.484986	2.894406
55	1	0	0.246098	-2.424116	4.741937
56	1	0	1.575902	2.593425	3.136150
57	1	0	1.345221	-0.697328	0.833678
58	6	0	0.177867	-8.426180	-3.047099
59	6	0	-0.912528	-10.197255	-3.971511
60	6	0	1.437227	-9.814484	-4.337869
61	6	0	0.294375	-10.599967	-4.570091
62	1	0	-1.835368	-10.748929	-4.103258
63	1	0	2.402725	-10.059106	-4.763688
64	1	0	0.342282	-11.486368	-5.189513
65	6	0	-0.177867	8.426180	-3.047099
66	6	0	0.912528	10.197255	-3.971511
67	6	0	-1.437227	9.814484	-4.337869
68	6	0	-0.294375	10.599967	-4.570091
69	1	0	1.835368	10.748929	-4.103258
70	1	0	-2.402725	10.059106	-4.763688
71	1	0	-0.342282	11.486368	-5.189513
72	7	0	1.374511	-8.704195	-3.559514
73	7	0	-0.968609	-9.086107	-3.193781
74	7	0	0.968609	9.086107	-3.193781
75	7	0	-1.374511	8.704195	-3.559514

Complex cation 5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.000000	0.000000	3.282466
2	7	0	2.157538	-0.205098	3.274968
3	7	0	-2.157538	0.205098	3.274968
4	7	0	-0.078967	-1.524025	4.853719
5	7	0	0.078967	1.524025	4.853719
6	1	0	-2.594306	0.092450	4.194920
7	1	0	2.594306	-0.092450	4.194920
8	1	0	-2.589519	-0.477655	2.644637
9	1	0	2.408463	-1.138040	2.933080
10	1	0	-2.408463	1.138040	2.933080
11	1	0	2.589519	0.477655	2.644637

12	1	0	0.208775	-2.432454	4.476267
13	1	0	-0.208775	2.432454	4.476267
14	1	0	-1.009842	-1.647508	5.263856
15	1	0	-0.556673	1.302545	5.626211
16	1	0	0.556673	-1.302545	5.626211
17	1	0	1.009842	1.647508	5.263856
18	7	0	-0.098384	-1.531989	1.860406
19	7	0	0.098384	1.531989	1.860406
20	6	0	0.730411	-1.584640	0.768871
21	6	0	0.932580	2.604406	2.035800
22	6	0	-0.932580	-2.604406	2.035800
23	6	0	-0.730411	1.584640	0.768871
24	6	0	-0.933854	-3.718675	1.200358
25	6	0	-0.789028	2.673599	-0.099188
26	6	0	0.789028	-2.673599	-0.099188
27	6	0	0.933854	3.718675	1.200358
28	6	0	-0.041074	-3.802452	0.106331
29	6	0	0.041074	3.802452	0.106331
30	6	0	-0.030043	-5.019559	-0.711002
31	6	0	0.030043	5.019559	-0.711002
32	6	0	0.857379	-5.325155	-1.694697
33	6	0	-0.857379	5.325155	-1.694697
34	6	0	0.873060	-6.567923	-2.475449
35	6	0	-0.873060	6.567923	-2.475449
36	6	0	-0.093454	-7.597173	-2.351817
37	6	0	-1.906590	6.775838	-3.417219
38	6	0	0.000000	-8.745136	-3.123389
39	6	0	-1.961106	7.944122	-4.169568
40	6	0	1.906590	-6.775838	-3.417219
41	6	0	0.093454	7.597173	-2.351817
42	6	0	1.961106	-7.944122	-4.169568
43	6	0	0.000000	8.745136	-3.123389
44	7	0	1.017809	-8.913833	-4.019037
45	7	0	-1.017809	8.913833	-4.019037
46	6	0	1.083073	-10.172423	-4.818044
47	6	0	-1.083073	10.172423	-4.818044
48	1	0	-1.607551	-2.567559	2.883145
49	1	0	-1.355501	0.715805	0.599171
50	1	0	1.355501	-0.715805	0.599171
51	1	0	1.607551	2.567559	2.883145
52	1	0	-1.621188	-4.530272	1.417060
53	1	0	-1.483090	2.625553	-0.930913
54	1	0	1.483090	-2.625553	-0.930913
55	1	0	1.621188	4.530272	1.417060
56	1	0	-0.807136	-5.737652	-0.454914
57	1	0	0.807136	5.737652	-0.454914
58	1	0	1.653103	-4.623896	-1.940257
59	1	0	-1.653103	4.623896	-1.940257
60	1	0	-0.926945	-7.524691	-1.664619
61	1	0	-2.681590	6.033644	-3.571146
62	1	0	2.681590	-6.033644	-3.571146
63	1	0	0.926945	7.524691	-1.664619
64	1	0	-0.721620	-9.549630	-3.050526
65	1	0	-2.745675	8.127082	-4.892707
66	1	0	2.745675	-8.127082	-4.892707
67	1	0	0.721620	9.549630	-3.050526
68	1	0	1.879621	-10.093592	-5.557477
69	1	0	-1.879621	10.093592	-5.557477
70	1	0	1.288869	-11.014671	-4.153603
71	1	0	-1.288869	11.014671	-4.153603
72	1	0	0.132632	-10.325992	-5.332740

73	1	0	-0.132632	10.325992	-5.332740

Complex cation 6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.225213	1.510798	2.980893
2	6	0	-0.595362	1.621145	1.887192
3	6	0	1.146209	2.511850	3.145119
4	6	0	1.241687	3.611765	2.296868
5	6	0	0.362412	3.757503	1.198089
6	6	0	-0.560213	2.699713	1.005688
7	7	0	-0.225213	-1.510798	2.980893
8	44	0	0.000000	0.000000	4.407745
9	6	0	-1.146209	-2.511850	3.145119
10	6	0	-1.241687	-3.611765	2.296868
11	6	0	-0.362412	-3.757503	1.198089
12	6	0	0.560213	-2.699713	1.005688
13	6	0	0.595362	-1.621145	1.887192
14	6	0	0.290754	-6.526790	-1.454560
15	6	0	1.265164	-6.767663	-2.451680
16	6	0	1.229602	-7.921263	-3.222360
17	7	0	0.239788	-8.848635	-3.050334
18	6	0	-0.727147	-8.642067	-2.101706
19	6	0	-0.716691	-7.510912	-1.301127
20	6	0	-0.290754	6.526790	-1.454560
21	6	0	0.716691	7.510912	-1.301127
22	6	0	0.727147	8.642067	-2.101706
23	7	0	-0.239788	8.848635	-3.050334
24	6	0	-1.229602	7.921263	-3.222360
25	6	0	-1.265164	6.767663	-2.451680
26	7	0	2.133852	-0.382987	4.397429
27	7	0	-0.201463	-1.514719	5.976104
28	7	0	0.201463	1.514719	5.976104
29	7	0	-2.133852	0.382987	4.397429
30	1	0	-1.290857	0.806051	1.724943
31	1	0	1.994746	4.365130	2.505105
32	1	0	-1.255919	2.699974	0.173953
33	1	0	-1.817299	-2.429027	3.992654
34	1	0	-1.994746	-4.365130	2.505105
35	1	0	1.255919	-2.699974	0.173953
36	1	0	2.074711	-6.066827	-2.621935
37	1	0	1.986844	-8.153824	-3.959341
38	1	0	-1.505007	-9.391665	-2.038803
39	1	0	-1.514617	-7.408108	-0.576165
40	1	0	1.514617	7.408108	-0.576165
41	1	0	1.505007	9.391665	-2.038803
42	1	0	-1.986844	8.153824	-3.959341
43	1	0	-2.074711	6.066827	-2.621935
44	1	0	2.579724	-0.319972	5.317715
45	1	0	2.305451	-1.328462	4.041230
46	1	0	0.452126	-1.346849	6.746774
47	1	0	-1.138428	-1.563153	6.387816
48	1	0	1.138428	1.563153	6.387816
49	1	0	-0.010291	2.441996	5.594386
50	1	0	-2.305451	1.328462	4.041230
51	1	0	-2.619458	-0.271037	3.775689
52	1	0	-2.579724	0.319972	5.317715
53	1	0	-0.452126	1.346849	6.746774

54	1	0	2.619458	0.271037	3.775689
55	1	0	0.010291	-2.441996	5.594386
56	1	0	1.817299	2.429027	3.992654
57	1	0	1.290857	-0.806051	1.724943
58	6	0	0.457051	4.958077	0.364655
59	6	0	-0.379571	5.304845	-0.650073
60	1	0	1.275878	5.625189	0.628287
61	1	0	-1.211258	4.651023	-0.908111
62	6	0	-0.457051	-4.958077	0.364655
63	6	0	0.379571	-5.304845	-0.650073
64	1	0	-1.275878	-5.625189	0.628287
65	1	0	1.211258	-4.651023	-0.908111
66	6	0	-0.211582	10.051300	-3.871674
67	6	0	-0.399286	9.934078	-5.258935
68	6	0	0.000000	11.295242	-3.254227
69	6	0	-0.373044	11.094833	-6.041283
70	1	0	-0.518575	8.963085	-5.731598
71	6	0	0.023508	12.445857	-4.051600
72	1	0	0.097777	11.380284	-2.175564
73	6	0	-0.162227	12.348222	-5.441373
74	1	0	-0.501503	11.021188	-7.115477
75	1	0	0.170456	13.415839	-3.589672
76	1	0	-0.143043	13.243613	-6.053009
77	6	0	0.211582	-10.051300	-3.871674
78	6	0	0.399286	-9.934078	-5.258935
79	6	0	0.000000	-11.295242	-3.254227
80	6	0	0.373044	-11.094833	-6.041283
81	1	0	0.518575	-8.963085	-5.731598
82	6	0	-0.023508	-12.445857	-4.051600
83	1	0	-0.097777	-11.380284	-2.175564
84	6	0	0.162227	-12.348222	-5.441373
85	1	0	0.501503	-11.021188	-7.115477
86	1	0	-0.170456	-13.415839	-3.589672
87	1	0	0.143043	-13.243613	-6.053009

Complex cation 7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.138018	1.524384	2.896481
2	6	0	-0.686962	1.589499	1.802556
3	6	0	0.995345	2.578931	3.067839
4	6	0	1.021588	3.689074	2.227800
5	6	0	0.132444	3.787727	1.131869
6	6	0	-0.720224	2.674829	0.929265
7	7	0	-0.138018	-1.524384	2.896481
8	44	0	0.000000	0.000000	4.320551
9	6	0	-0.995345	-2.578931	3.067839
10	6	0	-1.021588	-3.689074	2.227800
11	6	0	-0.132444	-3.787727	1.131869
12	6	0	0.720224	-2.674829	0.929265
13	6	0	0.686962	-1.589499	1.802556
14	6	0	0.726841	-6.551678	-1.465953
15	6	0	1.757751	-6.767558	-2.411892
16	6	0	1.804380	-7.932571	-3.162503
17	7	0	0.845325	-8.890602	-2.997380
18	6	0	-0.174735	-8.721625	-2.101138

19	6	0	-0.250095	-7.570384	-1.335578
20	6	0	-0.726841	6.551678	-1.465953
21	6	0	0.250095	7.570384	-1.335578
22	6	0	0.174735	8.721625	-2.101138
23	7	0	-0.845325	8.890602	-2.997380
24	6	0	-1.804380	7.932571	-3.162503
25	6	0	-1.757751	6.767558	-2.411892
26	7	0	2.151002	-0.263462	4.307431
27	7	0	-0.117776	-1.524247	5.889961
28	7	0	0.117776	1.524247	5.889961
29	7	0	-2.151002	0.263462	4.307431
30	1	0	-1.329038	0.732944	1.633860
31	1	0	1.725961	4.486827	2.441137
32	1	0	-1.412694	2.637211	0.095750
33	1	0	-1.670045	-2.530645	3.915015
34	1	0	-1.725961	-4.486827	2.441137
35	1	0	1.412694	-2.637211	0.095750
36	1	0	2.536977	-6.029842	-2.566349
37	1	0	2.567203	-8.161692	-3.896877
38	1	0	-0.883137	-9.539883	-2.051542
39	1	0	-1.079366	-7.485879	-0.644641
40	1	0	1.079366	7.485879	-0.644641
41	1	0	0.883137	9.539883	-2.051542
42	1	0	-2.567203	8.161692	-3.896877
43	1	0	-2.536977	6.029842	-2.566349
44	1	0	2.594955	-0.175971	5.226588
45	1	0	2.372675	-1.198289	3.950851
46	1	0	0.516904	-1.315698	6.666529
47	1	0	-1.053812	-1.631186	6.292571
48	1	0	1.053812	1.631186	6.292571
49	1	0	-0.155654	2.436161	5.510481
50	1	0	-2.372675	1.198289	3.950851
51	1	0	-2.598597	-0.415649	3.683990
52	1	0	-2.594955	0.175971	5.226588
53	1	0	-0.516904	1.315698	6.666529
54	1	0	2.598597	0.415649	3.683990
55	1	0	0.155654	-2.436161	5.510481
56	1	0	1.670045	2.530645	3.915015
57	1	0	1.329038	-0.732944	1.633860
58	6	0	0.145897	5.000696	0.310515
59	6	0	-0.730507	5.312897	-0.681449
60	1	0	0.930152	5.710101	0.568273
61	1	0	-1.532640	4.619733	-0.929845
62	6	0	-0.145897	-5.000696	0.310515
63	6	0	0.730507	-5.312897	-0.681449
64	1	0	-0.930152	-5.710101	0.568273
65	1	0	1.532640	-4.619733	-0.929845
66	6	0	-0.910892	10.121818	-3.790163
67	6	0	-2.001690	11.351145	-5.367720
68	6	0	0.000000	12.147477	-4.297140
69	6	0	-1.034975	12.360962	-5.223372
70	1	0	-2.830049	11.439652	-6.060151
71	1	0	0.782851	12.876847	-4.127974
72	1	0	-1.086086	13.271952	-5.805466
73	6	0	0.910892	-10.121818	-3.790163
74	6	0	2.001690	-11.351145	-5.367720
75	6	0	0.000000	-12.147477	-4.297140
76	6	0	1.034975	-12.360962	-5.223372
77	1	0	2.830049	-11.439652	-6.060151
78	1	0	-0.782851	-12.876847	-4.127974
79	1	0	1.086086	-13.271952	-5.805466

80	7	0	-0.061503	-11.005387	-3.567500
81	7	0	1.936436	-10.210464	-4.636412
82	7	0	0.061503	11.005387	-3.567500
83	7	0	-1.936436	10.210464	-4.636412

Complex cation 8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.000000	0.000000	4.079155
2	7	0	-0.295055	-1.501869	5.645531
3	7	0	0.295055	1.501869	5.645531
4	1	0	-0.177378	-2.439902	5.249930
5	1	0	0.177378	2.439902	5.249930
6	1	0	0.391443	-1.398848	6.398455
7	1	0	1.221333	1.470214	6.081842
8	1	0	-0.391443	1.398848	6.398455
9	1	0	-1.221333	-1.470214	6.081842
10	7	0	2.105114	-0.515549	4.063237
11	7	0	-2.105114	0.515549	4.063237
12	1	0	-2.559600	0.470686	4.980225
13	1	0	2.559600	-0.470686	4.980225
14	1	0	2.622114	0.104305	3.431926
15	1	0	-2.215895	1.472404	3.713483
16	1	0	2.215895	-1.472404	3.713483
17	1	0	-2.622114	-0.104305	3.431926
18	7	0	0.323126	1.491116	2.652098
19	7	0	-0.323126	-1.491116	2.652098
20	6	0	-0.488003	1.659940	1.558985
21	6	0	0.488003	-1.659940	1.558985
22	6	0	1.315126	2.422905	2.814938
23	6	0	-1.315126	-2.422905	2.814938
24	6	0	-0.375956	2.732285	0.676611
25	6	0	0.375956	-2.732285	0.676611
26	6	0	1.492166	3.509145	1.964999
27	6	0	-1.492166	-3.509145	1.964999
28	6	0	0.624048	3.719948	0.865620
29	6	0	-0.624048	-3.719948	0.865620
30	1	0	1.977456	2.293122	3.663814
31	1	0	-1.977456	-2.293122	3.663814
32	1	0	-1.238498	0.894671	1.398309
33	1	0	1.238498	-0.894671	1.398309
34	1	0	2.299159	4.205537	2.169200
35	1	0	-2.299159	-4.205537	2.169200
36	1	0	-1.067743	2.784782	-0.156866
37	1	0	1.067743	-2.784782	-0.156866
38	6	0	0.812747	4.904215	0.035319
39	6	0	-0.812747	-4.904215	0.035319
40	1	0	-1.694691	-5.497364	0.276576
41	1	0	1.694691	5.497364	0.276576
42	6	0	0.000000	5.356374	-0.965332
43	6	0	0.000000	-5.356374	-0.965332
44	1	0	0.907047	-4.817052	-1.237224
45	1	0	-0.907047	4.817052	-1.237224
46	6	0	0.281151	6.577385	-1.690495
47	6	0	-0.281151	-6.577385	-1.690495
48	1	0	-1.194729	-7.102107	-1.412485

49	1	0	1.194729	7.102107	-1.412485
50	6	0	-0.536301	7.082055	-2.660745
51	6	0	0.536301	-7.082055	-2.660745
52	1	0	1.446246	-6.537056	-2.908495
53	1	0	-1.446246	6.537056	-2.908495
54	6	0	-0.321222	8.315837	-3.411041
55	6	0	0.321222	-8.315837	-3.411041
56	6	0	-0.814936	-9.153209	-3.260032
57	6	0	0.814936	9.153209	-3.260032
58	6	0	-1.292736	8.729595	-4.354673
59	6	0	1.292736	-8.729595	-4.354673
60	1	0	-2.187136	8.141727	-4.526325
61	1	0	2.187136	-8.141727	-4.526325
62	1	0	-1.611452	-8.914863	-2.566663
63	1	0	1.611452	8.914863	-2.566663
64	6	0	-1.126363	9.900576	-5.082001
65	6	0	1.126363	-9.900576	-5.082001
66	6	0	-0.938699	-10.311850	-4.007877
67	6	0	0.938699	10.311850	-4.007877
68	1	0	1.792762	10.971241	-3.914143
69	1	0	-1.792762	-10.971241	-3.914143
70	1	0	1.857449	-10.237354	-5.805771
71	1	0	-1.857449	10.237354	-5.805771
72	7	0	0.022476	-10.680333	-4.907570
73	7	0	-0.022476	10.680333	-4.907570
74	6	0	-0.146868	-11.945242	-5.676049
75	6	0	0.146868	11.945242	-5.676049
76	1	0	-0.060988	-12.798327	-4.999104
77	1	0	0.060988	12.798327	-4.999104
78	1	0	0.626444	-12.013569	-6.440805
79	1	0	1.125526	11.950069	-6.159724
80	1	0	-0.626444	12.013569	-6.440805
81	1	0	-1.125526	-11.950069	-6.159724

Complex cation 9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.290103	1.497383	3.754397
2	6	0	-0.518058	1.644624	2.655752
3	6	0	1.253645	2.457499	3.925001
4	6	0	1.402320	3.551542	3.080321
5	6	0	0.536305	3.739373	1.974648
6	6	0	-0.431231	2.721145	1.776091
7	7	0	-0.290103	-1.497383	3.754397
8	44	0	0.000000	0.000000	5.180551
9	6	0	-1.253645	-2.457499	3.925001
10	6	0	-1.402320	-3.551542	3.080321
11	6	0	-0.536305	-3.739373	1.974648
12	6	0	0.431231	-2.721145	1.776091
13	6	0	0.518058	-1.644624	2.655752
14	6	0	0.488417	-8.270134	-2.351525
15	6	0	1.398182	-8.589302	-3.389673
16	6	0	1.279144	-9.770584	-4.105387
17	7	0	0.287729	-10.667985	-3.818066
18	6	0	-0.608592	-10.394036	-2.818428
19	6	0	-0.533575	-9.218624	-2.090657

20	6	0	-0.488417	8.270134	-2.351525
21	6	0	0.533575	9.218624	-2.090657
22	6	0	0.608592	10.394036	-2.818428
23	7	0	-0.287729	10.667985	-3.818066
24	6	0	-1.279144	9.770584	-4.105387
25	6	0	-1.398182	8.589302	-3.389673
26	7	0	2.116417	-0.465886	5.159751
27	7	0	-0.259318	-1.509420	6.746940
28	7	0	0.259318	1.509420	6.746940
29	7	0	-2.116417	0.465886	5.159751
30	1	0	-1.245896	0.858920	2.489125
31	1	0	2.186229	4.271691	3.291814
32	1	0	-1.120841	2.756177	0.939924
33	1	0	-1.915739	-2.343748	4.776433
34	1	0	-2.186229	-4.271691	3.291814
35	1	0	1.120841	-2.756177	0.939924
36	1	0	2.199182	-7.908303	-3.654299
37	1	0	1.935186	-10.023709	-4.927676
38	1	0	-1.347870	-11.157783	-2.616128
39	1	0	-1.266462	-9.065672	-1.308481
40	1	0	1.266462	9.065672	-1.308481
41	1	0	1.347870	11.157783	-2.616128
42	1	0	-1.935186	10.023709	-4.927676
43	1	0	-2.199182	7.908303	-3.654299
44	1	0	2.572295	-0.419343	6.075845
45	1	0	2.247248	-1.416460	4.800050
46	1	0	0.422171	-1.387136	7.501397
47	1	0	-1.187541	-1.502989	7.180106
48	1	0	1.187541	1.502989	7.180106
49	1	0	0.114584	2.443414	6.350791
50	1	0	-2.247248	1.416460	4.800050
51	1	0	-2.616265	-0.172073	4.532706
52	1	0	-2.572295	0.419343	6.075845
53	1	0	-0.422171	1.387136	7.501397
54	1	0	2.616265	0.172073	4.532706
55	1	0	-0.114584	-2.443414	6.350791
56	1	0	1.915739	2.343748	4.776433
57	1	0	1.245896	-0.858920	2.489125
58	6	0	0.690757	4.933277	1.153382
59	6	0	-0.098408	5.335584	0.112764
60	1	0	1.523003	5.578529	1.434052
61	1	0	-0.951368	4.737153	-0.206803
62	6	0	-0.690757	-4.933277	1.153382
63	6	0	0.098408	-5.335584	0.112764
64	1	0	-1.523003	-5.578529	1.434052
65	1	0	0.951368	-4.737153	-0.206803
66	6	0	0.136560	6.574431	-0.596346
67	6	0	-0.652999	7.019417	-1.617793
68	1	0	0.990407	7.164240	-0.264454
69	1	0	-1.497559	6.404313	-1.926428
70	6	0	-0.136560	-6.574431	-0.596346
71	6	0	0.652999	-7.019417	-1.617793
72	1	0	-0.990407	-7.164240	-0.264454
73	1	0	1.497559	-6.404313	-1.926428
74	6	0	0.187885	-11.914099	-4.566352
75	6	0	-1.061865	-12.313523	-5.066019
76	6	0	1.345290	-12.683303	-4.765678
77	6	0	-1.147941	-13.514617	-5.781262
78	1	0	-1.942688	-11.689839	-4.941668
79	6	0	1.242510	-13.880371	-5.485430
80	1	0	2.298691	-12.385688	-4.338281

81	6	0	0.000000	-14.296937	-5.991971
82	1	0	-2.103303	-13.831298	-6.184963
83	1	0	2.124713	-14.492372	-5.637361
84	1	0	-0.073341	-15.225421	-6.547621
85	6	0	-0.187885	11.914099	-4.566352
86	6	0	1.061865	12.313523	-5.066019
87	6	0	-1.345290	12.683303	-4.765678
88	6	0	1.147941	13.514617	-5.781262
89	1	0	1.942688	11.689839	-4.941668
90	6	0	-1.242510	13.880371	-5.485430
91	1	0	-2.298691	12.385688	-4.338281
92	6	0	0.000000	14.296937	-5.991971
93	1	0	2.103303	13.831298	-6.184963
94	1	0	-2.124713	14.492372	-5.637361
95	1	0	0.073341	15.225421	-6.547621

Complex cation 10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.321681	1.488051	3.387358
2	6	0	-0.488634	1.656001	2.293021
3	6	0	1.313019	2.421435	3.549791
4	6	0	1.488853	3.506983	2.701066
5	6	0	0.620108	3.719559	1.600189
6	6	0	-0.378256	2.727846	1.411348
7	7	0	-0.321681	-1.488051	3.387358
8	44	0	0.000000	0.000000	4.814732
9	6	0	-1.313019	-2.421435	3.549791
10	6	0	-1.488853	-3.506983	2.701066
11	6	0	-0.620108	-3.719559	1.600189
12	6	0	0.378256	-2.727846	1.411348
13	6	0	0.488634	-1.656001	2.293021
14	6	0	0.769844	-10.161428	-4.245701
15	6	0	1.710287	-10.616946	-5.206587
16	6	0	1.514067	-11.807726	-5.885685
17	7	0	0.409928	-12.576558	-5.650604
18	6	0	-0.518214	-12.171501	-4.733558
19	6	0	-0.363979	-10.988100	-4.030524
20	6	0	0.244161	-13.862398	-6.380692
21	6	0	-0.769844	10.161428	-4.245701
22	6	0	0.363979	10.988100	-4.030524
23	6	0	0.518214	12.171501	-4.733558
24	7	0	-0.409928	12.576558	-5.650604
25	6	0	-1.514067	11.807726	-5.885685
26	6	0	-1.710287	10.616946	-5.206587
27	6	0	-0.244161	13.862398	-6.380692
28	7	0	2.104987	-0.512337	4.789800
29	7	0	-0.293375	-1.507999	6.377404
30	7	0	0.293375	1.507999	6.377404
31	7	0	-2.104987	0.512337	4.789800
32	1	0	-1.236301	0.888055	2.130887
33	1	0	2.294908	4.204668	2.904432
34	1	0	-1.069124	2.779683	0.577068
35	1	0	-1.975718	-2.291558	4.398738
36	1	0	-2.294908	-4.204668	2.904432
37	1	0	1.069124	-2.779683	0.577068

38	1	0	2.601090	-10.039488	-5.425747
39	1	0	2.218145	-12.176653	-6.621173
40	1	0	-1.372664	-12.819733	-4.586757
41	1	0	-1.135400	-10.721710	-3.319383
42	1	0	0.426838	-13.704492	-7.445066
43	1	0	0.947531	-14.600906	-5.988726
44	1	0	-0.774153	-14.227748	-6.248734
45	1	0	1.135400	10.721710	-3.319383
46	1	0	1.372664	12.819733	-4.586757
47	1	0	-2.218145	12.176653	-6.621173
48	1	0	-2.601090	10.039488	-5.425747
49	1	0	0.774153	14.227748	-6.248734
50	1	0	-0.426838	13.704492	-7.445066
51	1	0	-0.947531	14.600906	-5.988726
52	1	0	2.566067	-0.469889	5.703337
53	1	0	2.211829	-1.467357	4.434122
54	1	0	0.401072	-1.415756	7.124024
55	1	0	-1.215810	-1.471205	6.820842
56	1	0	1.215810	1.471205	6.820842
57	1	0	0.186998	2.442310	5.970148
58	1	0	-2.211829	1.467357	4.434122
59	1	0	-2.613247	-0.111974	4.155882
60	1	0	-2.566067	0.469889	5.703337
61	1	0	-0.401072	1.415756	7.124024
62	1	0	2.613247	0.111974	4.155882
63	1	0	-0.186998	-2.442310	5.970148
64	1	0	1.975718	2.291558	4.398738
65	1	0	1.236301	-0.888055	2.130887
66	6	0	0.806424	4.902423	0.776362
67	6	0	0.000000	5.354866	-0.233301
68	1	0	1.680130	5.503800	1.026456
69	1	0	-0.900002	4.809499	-0.517579
70	6	0	-0.806424	-4.902423	0.776362
71	6	0	0.000000	-5.354866	-0.233301
72	1	0	-1.680130	-5.503800	1.026456
73	1	0	0.900002	-4.809499	-0.517579
74	6	0	0.281135	6.578187	-0.943337
75	6	0	-0.517261	7.107931	-1.924618
76	1	0	1.187375	7.114376	-0.658971
77	1	0	-1.428806	6.587457	-2.218867
78	6	0	-0.281135	-6.578187	-0.943337
79	6	0	0.517261	-7.107931	-1.924618
80	1	0	-1.187375	-7.114376	-0.658971
81	1	0	1.428806	-6.587457	-2.218867
82	6	0	0.212418	-8.350741	-2.589756
83	6	0	1.012329	-8.906770	-3.550411
84	1	0	-0.705590	-8.850630	-2.281508
85	1	0	1.923920	-8.381203	-3.830855
86	6	0	-0.212418	8.350741	-2.589756
87	6	0	-1.012329	8.906770	-3.550411
88	1	0	0.705590	8.850630	-2.281508
89	1	0	-1.923920	8.381203	-3.830855

Complex cation 11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	0.288260	1.488749	4.025205
2	6	0	-0.520579	1.619853	2.924689
3	6	0	1.253206	2.450766	4.177268
4	6	0	1.405295	3.527169	3.311916
5	6	0	0.539938	3.699374	2.201342
6	6	0	-0.431000	2.677849	2.026008
7	7	0	-0.288260	-1.488749	4.025205
8	44	0	0.000000	0.000000	5.458023
9	6	0	-1.253206	-2.450766	4.177268
10	6	0	-1.405295	-3.527169	3.311916
11	6	0	-0.539938	-3.699374	2.201342
12	6	0	0.431000	-2.677849	2.026008
13	6	0	0.520579	-1.619853	2.924689
14	7	0	2.115328	-0.465400	5.427507
15	7	0	-0.262010	-1.519370	7.016288
16	7	0	0.262010	1.519370	7.016288
17	7	0	-2.115328	0.465400	5.427507
18	1	0	-1.247968	0.831176	2.769938
19	1	0	2.191334	4.249061	3.509047
20	1	0	-1.118004	2.694968	1.187308
21	1	0	-1.915352	-2.351197	5.031065
22	1	0	-2.191334	-4.249061	3.509047
23	1	0	1.118004	-2.694968	1.187308
24	1	0	2.576500	-0.429013	6.341056
25	1	0	2.240026	-1.411462	5.054316
26	1	0	0.426662	-1.412326	7.766035
27	1	0	-1.187509	-1.507045	7.454313
28	1	0	1.187509	1.507045	7.454313
29	1	0	0.129948	2.447874	6.603465
30	1	0	-2.240026	1.411462	5.054316
31	1	0	-2.607580	-0.181280	4.803440
32	1	0	-2.576500	0.429013	6.341056
33	1	0	-0.426662	1.412326	7.766035
34	1	0	2.607580	0.181280	4.803440
35	1	0	-0.129948	-2.447874	6.603465
36	1	0	1.915352	2.351197	5.031065
37	1	0	1.247968	-0.831176	2.769938
38	6	0	0.695986	4.869498	1.351509
39	6	0	-0.132691	5.244915	0.335010
40	1	0	1.546748	5.501640	1.597032
41	1	0	-1.002511	4.627686	0.107934
42	6	0	-0.695986	-4.869498	1.351509
43	6	0	0.132691	-5.244915	0.335010
44	1	0	-1.546748	-5.501640	1.597032
45	1	0	1.002511	-4.627686	0.107934
46	6	0	0.000000	-6.439692	-0.493788
47	6	0	-1.089671	-7.339337	-0.397461
48	6	0	1.016345	-6.727438	-1.439635
49	6	0	-1.145789	-8.474252	-1.201662
50	1	0	-1.899166	-7.155739	0.301587
51	6	0	0.962580	-7.865125	-2.241347
52	1	0	1.860501	-6.049565	-1.536969
53	6	0	-0.121266	-8.770350	-2.135968
54	1	0	-1.991937	-9.149948	-1.108620
55	1	0	1.765983	-8.045660	-2.948021
56	6	0	0.000000	6.439692	-0.493788
57	6	0	1.089671	7.339337	-0.397461
58	6	0	-1.016345	6.727438	-1.439635
59	6	0	1.145789	8.474252	-1.201662
60	1	0	1.899166	7.155739	0.301587
61	6	0	-0.962580	7.865125	-2.241347

62	1	0	-1.860501	6.049565	-1.536969
63	6	0	0.121266	8.770350	-2.135968
64	1	0	1.991937	9.149948	-1.108620
65	1	0	-1.765983	8.045660	-2.948021
66	6	0	-0.239696	-9.989138	-2.930750
67	6	0	0.659685	-10.460697	-3.840932
68	1	0	-1.149288	-10.560416	-2.746381
69	1	0	1.574545	-9.902696	-4.026940
70	6	0	0.239696	9.989138	-2.930750
71	6	0	-0.659685	10.460697	-3.840932
72	1	0	1.149288	10.560416	-2.746381
73	1	0	-1.574545	9.902696	-4.026940
74	6	0	-0.517073	11.686447	-4.610994
75	6	0	-1.545031	12.063401	-5.514270
76	6	0	0.597292	12.564221	-4.526447
77	6	0	-1.450492	13.226524	-6.259934
78	1	0	-2.428257	11.446639	-5.633989
79	6	0	0.648792	13.715969	-5.290845
80	1	0	1.431337	12.362826	-3.866463
81	7	0	-0.364388	14.046051	-6.147878
82	1	0	-2.223626	13.531534	-6.953755
83	1	0	1.486905	14.399945	-5.244021
84	6	0	0.517073	-11.686447	-4.610994
85	6	0	1.545031	-12.063401	-5.514270
86	6	0	-0.597292	-12.564221	-4.526447
87	6	0	1.450492	-13.226524	-6.259934
88	1	0	2.428257	-11.446639	-5.633989
89	6	0	-0.648792	-13.715969	-5.290845
90	1	0	-1.431337	-12.362826	-3.866463
91	7	0	0.364388	-14.046051	-6.147878
92	1	0	2.223626	-13.531534	-6.953755
93	1	0	-1.486905	-14.399945	-5.244021
94	6	0	-0.262903	15.272540	-6.982298
95	1	0	0.294861	16.037287	-6.440402
96	1	0	0.247410	15.039979	-7.920283
97	1	0	-1.262726	15.653364	-7.193524
98	6	0	0.262903	-15.272540	-6.982298
99	1	0	-0.247410	-15.039979	-7.920283
100	1	0	1.262726	-15.653364	-7.193524
101	1	0	-0.294861	-16.037287	-6.440402

4. Complete Reference

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